



## wwPDB EM Validation Summary Report ⓘ

Sep 15, 2021 – 01:33 pm BST

PDB ID : 7OY8  
EMDB ID : EMD-13110  
Title : Cryo-EM structure of the Rhodospirillum rubrum RC-LH1 complex  
Authors : Qian, P.; Croll, T.I.; Castro, H.P.; Moriarty, N.W.; sader, K.; Hunter, C.N.  
Deposited on : 2021-06-23  
Resolution : 2.50 Å(reported)  
Based on initial models : 1LGH, 3I4D

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

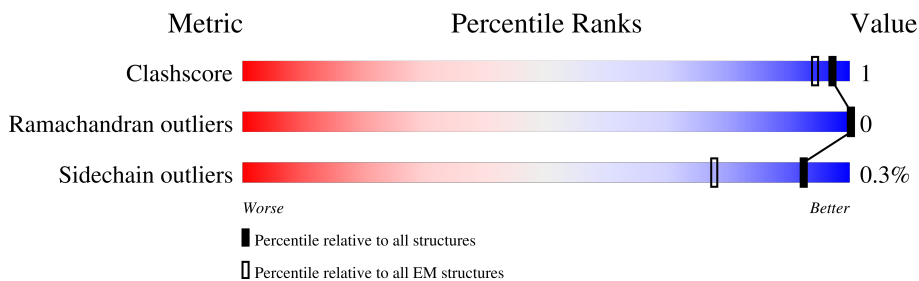
EMDB validation analysis : 0.0.0.dev97  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.1

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	54	81% (green), 19% (grey)
1	3	54	81% (green), 19% (grey)
1	5	54	81% (green), 19% (grey), 1% (red), 1% (orange)
1	7	54	80% (green), 19% (grey), 1% (red), 1% (orange), 1% (yellow)
1	9	54	85% (green), 15% (grey), 1% (red), 1% (orange)
1	I	54	80% (green), 19% (grey), 1% (yellow)
1	K	54	83% (green), 17% (grey)
1	O	54	81% (green), 19% (grey)

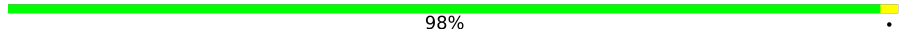

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Mol	Chain	Length	Quality of chain
1	Q	54	87% 13%
1	S	54	83% 17%
1	U	54	81% 19%
1	W	54	81% 19%
1	Y	54	76% 20%
1	d	54	81% 19%
1	m	54	83% 17%
1	n	54	81% 19%
2	2	50	92% 8%
2	4	50	6% 94% 6%
2	6	50	90% 6%
2	8	50	94% 6%
2	A	50	86% 6% 8%
2	D	50	90% 6%
2	E	50	90% 8%
2	F	50	92% 6%
2	G	50	94% 6%
2	J	50	90% 8%
2	N	50	90% 8%
2	T	50	94% 6%
2	V	50	92% 8%
2	X	50	92% 6%
2	Z	50	94% 6%
3	H	257	100%
4	L	276	96%

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Mol	Chain	Length	Quality of chain
5	M	306	 98%
6	R	62	 5% 71% 26%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	07D	1	1001	X	-	-	-
7	07D	2	1001	X	-	-	-
7	07D	3	102	X	-	-	-
7	07D	4	1001	X	-	-	-
7	07D	5	102	X	-	-	-
7	07D	6	1001	X	-	-	-
7	07D	7	102	X	-	-	-
7	07D	8	1001	X	-	-	-
7	07D	9	102	X	-	-	-
7	07D	A	101	X	-	-	-
7	07D	D	1001	X	-	-	-
7	07D	E	1001	X	-	-	-
7	07D	F	1001	X	-	-	-
7	07D	G	1001	X	-	-	-
7	07D	H	301	X	-	-	-
7	07D	I	102	X	-	-	-
7	07D	J	1001	X	-	-	-
7	07D	K	102	X	-	-	-
7	07D	L	1004	X	-	-	-
7	07D	L	1005	X	-	-	-
7	07D	M	404	X	-	-	-
7	07D	M	405	X	-	-	-
7	07D	N	1002	X	-	-	-
7	07D	O	102	X	-	-	-
7	07D	Q	102	X	-	-	-
7	07D	R	101	X	-	-	-
7	07D	S	102	X	-	-	-
7	07D	T	101	X	-	-	-
7	07D	U	1001	X	-	-	-
7	07D	V	1001	X	-	-	-
7	07D	W	1001	X	-	-	-
7	07D	X	1001	X	-	-	-
7	07D	Y	102	X	-	-	-

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<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
7	07D	Z	1001	X	-	-	-
7	07D	d	1002	X	-	-	-
7	07D	m	102	X	-	-	-
7	07D	n	102	X	-	-	-

## 2 Entry composition i

There are 18 unique types of molecules in this entry. The entry contains 22902 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Light-harvesting protein B-870 beta chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	1	44	360	247	57	56	0	0
1	3	44	360	247	57	56	0	0
1	5	44	360	247	57	56	0	0
1	7	44	360	247	57	56	0	0
1	9	46	370	252	59	59	0	0
1	I	44	360	247	57	56	0	0
1	K	45	364	249	58	57	0	0
1	O	44	360	247	57	56	0	0
1	Q	47	378	258	60	60	0	0
1	S	45	364	249	58	57	0	0
1	U	44	360	247	57	56	0	0
1	W	44	360	247	57	56	0	0
1	Y	43	352	241	56	55	0	0
1	d	44	360	247	57	56	0	0
1	m	45	364	249	58	57	0	0
1	n	44	360	247	57	56	0	0

- Molecule 2 is a protein called Antenna complex, alpha/beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	46	Total	C	N	O	S	0	0
			388	263	63	61	1		
2	4	47	Total	C	N	O	S	0	0
			397	269	65	62	1		
2	6	47	Total	C	N	O	S	0	0
			397	269	65	62	1		
2	8	48	Total	C	N	O	S	0	0
			404	274	66	63	1		
2	A	46	Total	C	N	O	S	0	0
			388	263	63	61	1		
2	D	47	Total	C	N	O	S	0	0
			397	269	65	62	1		
2	E	46	Total	C	N	O	S	0	0
			388	263	63	61	1		
2	F	47	Total	C	N	O	S	0	0
			397	269	65	62	1		
2	G	47	Total	C	N	O	S	0	0
			397	269	65	62	1		
2	J	46	Total	C	N	O	S	0	0
			388	263	63	61	1		
2	N	46	Total	C	N	O	S	0	0
			388	263	63	61	1		
2	T	47	Total	C	N	O	S	0	0
			397	269	65	62	1		
2	V	46	Total	C	N	O	S	0	0
			388	263	63	61	1		
2	X	47	Total	C	N	O	S	0	0
			397	269	65	62	1		
2	Z	47	Total	C	N	O	S	0	0
			397	269	65	62	1		

- Molecule 3 is a protein called Photosynthetic reaction center, H-chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	257	Total	C	N	O	S	0	0
			1972	1263	343	362	4		

- Molecule 4 is a protein called Photosynthetic reaction center L subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	274	Total	C	N	O	S	0	0
			2164	1456	344	354	10		

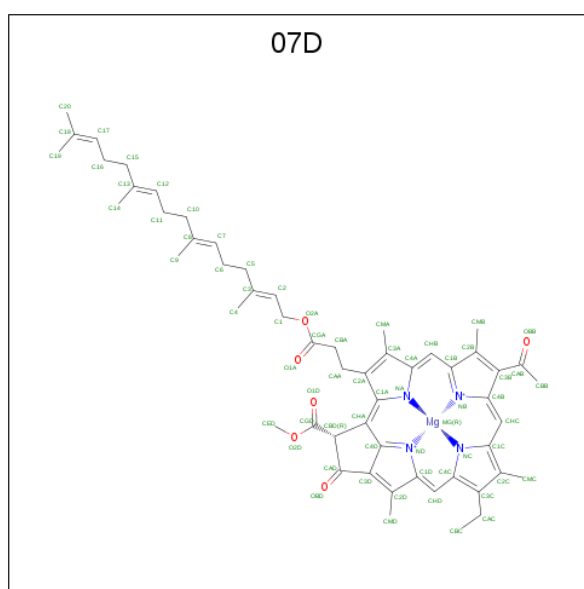
- Molecule 5 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	M	305	2424	1619	398	398	9	0	0

- Molecule 6 is a protein called Antenna complex, alpha/beta subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	R	46	387	263	64	60	0	0

- Molecule 7 is Trans-Geranyl BACTERIOCHLOROPHYLL A (three-letter code: 07D) (formula:  $C_{55}H_{64}MgN_4O_6$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
7	1	1	66	55	1	4	6	0
7	2	1	66	55	1	4	6	0
7	3	1	66	55	1	4	6	0
7	4	1	66	55	1	4	6	0
7	5	1	66	55	1	4	6	0
7	6	1	66	55	1	4	6	0
7	7	1	66	55	1	4	6	0

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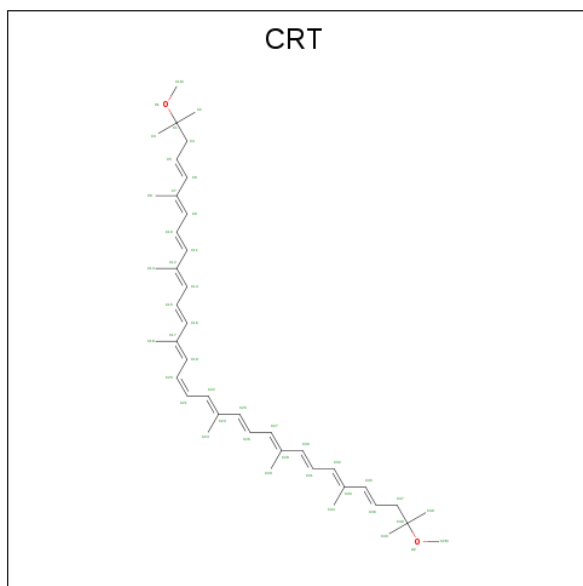
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
7	8	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	9	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	D	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	E	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	F	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	H	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	I	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	J	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	K	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	L	1	Total 132	C 110	Mg 2	N 8	O 12	0
7	L	1	Total 132	C 110	Mg 2	N 8	O 12	0
7	M	1	Total 132	C 110	Mg 2	N 8	O 12	0
7	M	1	Total 132	C 110	Mg 2	N 8	O 12	0
7	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	O	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	R	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	S	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	T	1	Total 66	C 55	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
7	U	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	V	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	W	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	X	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	Z	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	d	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	m	1	Total 66	C 55	Mg 1	N 4	O 6	0
7	n	1	Total 66	C 55	Mg 1	N 4	O 6	0

- Molecule 8 is SPIRILLOXANTHIN (three-letter code: CRT) (formula: C<sub>42</sub>H<sub>60</sub>O<sub>2</sub>).



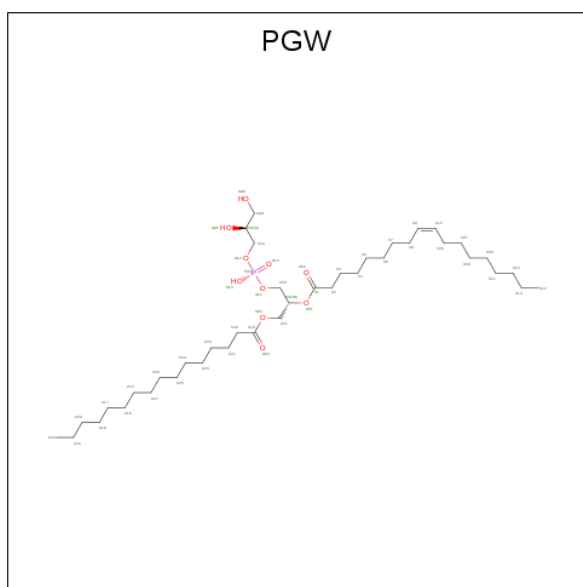
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
8	1	1	Total 44	C 42	O 2	0
8	3	1	Total 44	C 42	O 2	0

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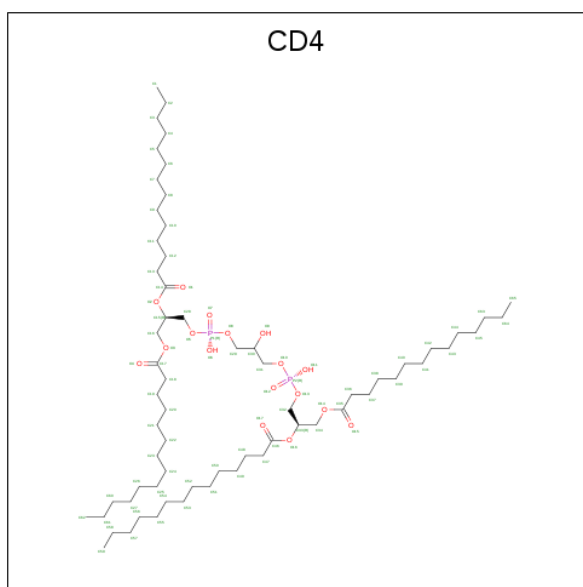
Mol	Chain	Residues	Atoms			AltConf
8	5	1	Total	C	O	0
			44	42	2	
8	7	1	Total	C	O	0
			44	42	2	
8	9	1	Total	C	O	0
			44	42	2	
8	I	1	Total	C	O	0
			44	42	2	
8	J	1	Total	C	O	0
			44	42	2	
8	K	1	Total	C	O	0
			44	42	2	
8	M	1	Total	C	O	0
			44	42	2	
8	N	1	Total	C	O	0
			44	42	2	
8	O	1	Total	C	O	0
			44	42	2	
8	Q	1	Total	C	O	0
			44	42	2	
8	S	1	Total	C	O	0
			44	42	2	
8	Y	1	Total	C	O	0
			44	42	2	
8	d	1	Total	C	O	0
			44	42	2	
8	m	1	Total	C	O	0
			44	42	2	
8	n	1	Total	C	O	0
			44	42	2	

- Molecule 9 is (1R)-2-[[[S]-[[[2S)-2,3-dihydroxypropyl]oxy](hydroxy)phosphoryl]oxy]-1-[(hexadecanoyloxy)methyl]ethyl (9Z)-octadec-9-enoate (three-letter code: PGW) (formula: C<sub>40</sub>H<sub>77</sub>O<sub>10</sub>P).



Mol	Chain	Residues	Atoms			AltConf	
			Total	C	O		P
9	H	1	102	80	20	2	0
9	H	1	102	80	20	2	0

- Molecule 10 is (2R,5R,11R,14R)-5,8,11-trihydroxy-5,11-dioxido-17-oxo-2,14-bis(tetradecano yloxy)-4,6,10,12,16-pentaoxa-5,11-diphosphatriacont-1-yl tetradecanoate (three-letter code: CD4) (formula:  $C_{65}H_{126}O_{17}P_2$ ).



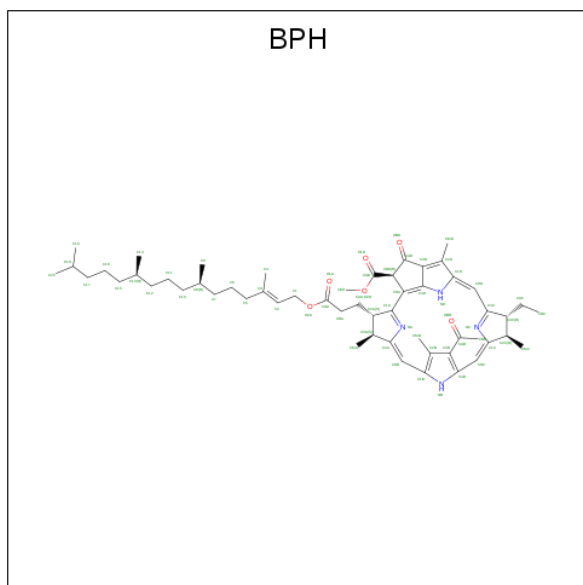
Mol	Chain	Residues	Atoms			AltConf	
			Total	C	O		P
10	H	1	84	65	17	2	0

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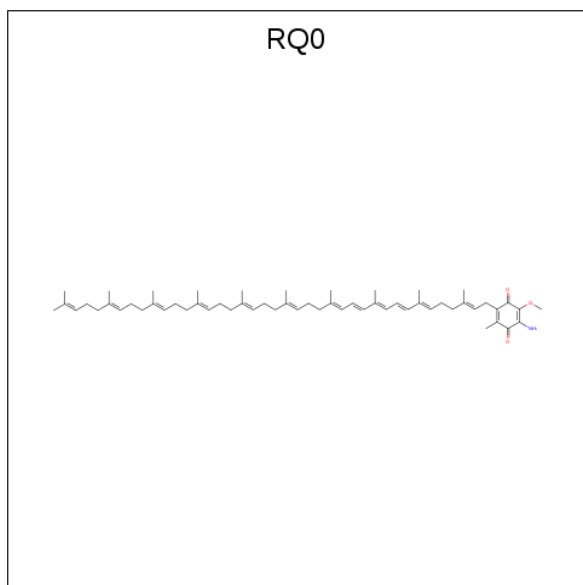
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
10	M	1	84	65	17	2	0

- Molecule 11 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula:  $C_{55}H_{76}N_4O_6$ ) (labeled as "Ligand of Interest" by depositor).



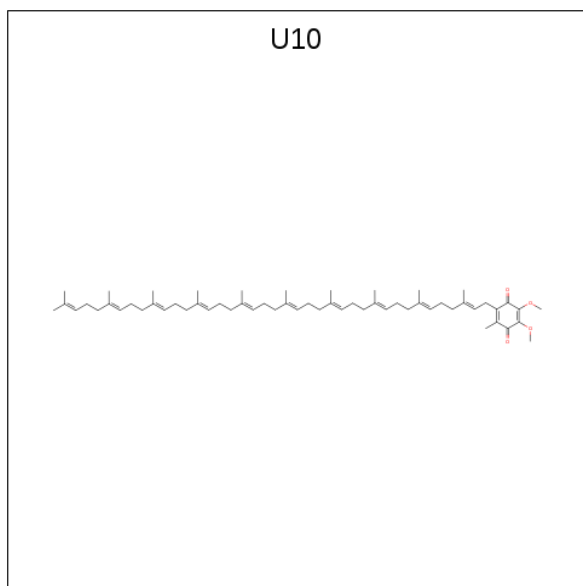
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
11	L	1	65	55	4	6	0
11	M	1	65	55	4	6	0

- Molecule 12 is 2-azanyl-5-[(2 {E},6 {E},8 {E},10 {E},12 {E},14 {E},18 {E},22 {E},26 {E},30 {E},34 {E})-3,7,11,15,19,23,27,31,35,39-decamethyltetraconta-2,6,8,10,12,14,18,22,26,30,34,38-dodecaenyl]-3-methoxy-6-methyl-cyclohexa-2,5-diene-1,4-dione (three-letter code: RQ0) (formula:  $C_{58}H_{85}NO_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
12	L	1	62	58	1	3	0

- Molecule 13 is UBIQUINONE-10 (three-letter code: U10) (formula: C<sub>59</sub>H<sub>90</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
13	L	1	126	118	8	0
13	L	1	126	118	8	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
13	M	1	63	59	4	0

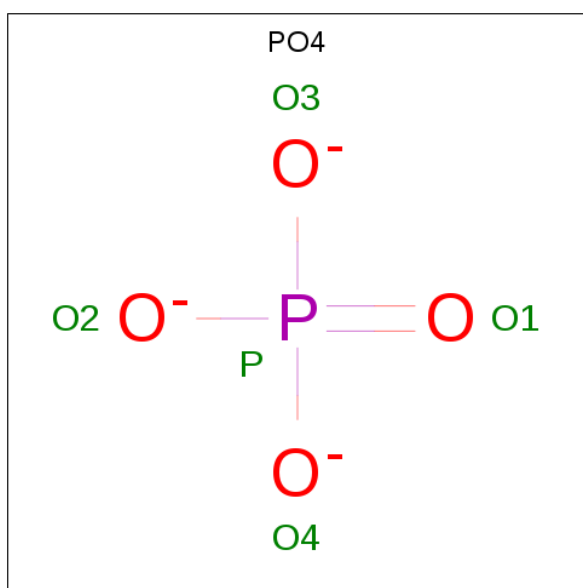
- Molecule 14 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
			Total	Fe	
14	M	1	1	1	0

- Molecule 15 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

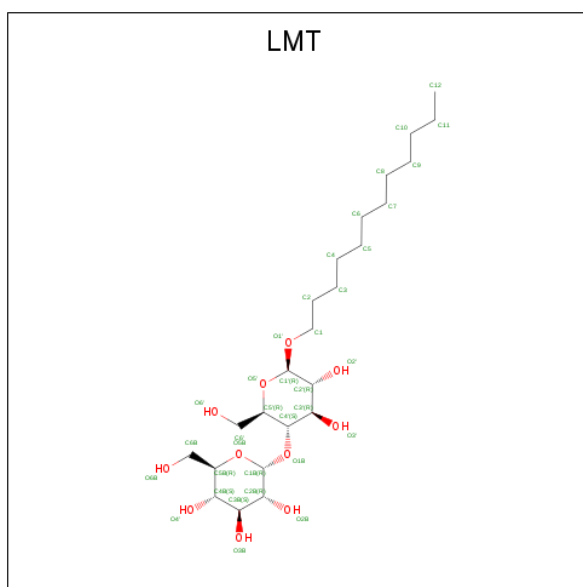
Mol	Chain	Residues	Atoms		AltConf
			Total	Cl	
15	M	1	1	1	0

- Molecule 16 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			AltConf
			Total	O	P	
16	M	1	5	4	1	0

- Molecule 17 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
17	R	1	35	24	11	0

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		AltConf
18	2	1	Total	O	0
			1	1	
18	3	1	Total	O	0
			1	1	
18	4	11	Total	O	0
			11	11	
18	5	2	Total	O	0
			2	2	
18	6	8	Total	O	0
			8	8	
18	7	1	Total	O	0
			1	1	
18	8	6	Total	O	0
			6	6	
18	9	1	Total	O	0
			1	1	
18	A	8	Total	O	0
			8	8	
18	D	6	Total	O	0
			6	6	
18	E	5	Total	O	0
			5	5	

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Mol	Chain	Residues	Atoms		AltConf
18	F	6	Total 6	O 6	0
18	G	8	Total 8	O 8	0
18	H	68	Total 68	O 68	0
18	I	1	Total 1	O 1	0
18	J	3	Total 3	O 3	0
18	K	1	Total 1	O 1	0
18	L	89	Total 89	O 89	0
18	M	86	Total 86	O 86	0
18	N	14	Total 14	O 14	0
18	O	3	Total 3	O 3	0
18	Q	2	Total 2	O 2	0
18	R	8	Total 8	O 8	0
18	S	2	Total 2	O 2	0
18	T	4	Total 4	O 4	0
18	U	3	Total 3	O 3	0
18	V	4	Total 4	O 4	0
18	W	1	Total 1	O 1	0
18	X	8	Total 8	O 8	0
18	Y	1	Total 1	O 1	0
18	Z	7	Total 7	O 7	0
18	d	2	Total 2	O 2	0

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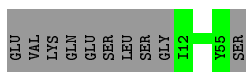
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>AltConf</b>
18	n	1	Total	O	0
			1	1	

### 3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

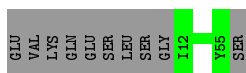
- Molecule 1: Light-harvesting protein B-870 beta chain

Chain 1:  81% 19%




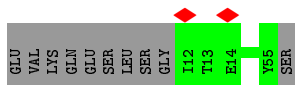
- Molecule 1: Light-harvesting protein B-870 beta chain

Chain 3:  81% 19%




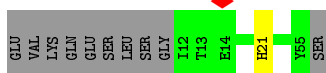
- Molecule 1: Light-harvesting protein B-870 beta chain

Chain 5:  81% 19%




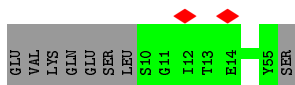
- Molecule 1: Light-harvesting protein B-870 beta chain

Chain 7:  80% 19%




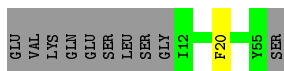
- Molecule 1: Light-harvesting protein B-870 beta chain

Chain 9:  85% 15%




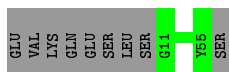
- Molecule 1: Light-harvesting protein B-870 beta chain

Chain I:  80% 19%




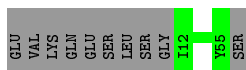
- Molecule 1: Light-harvesting protein B-870 beta chain

Chain K:  83% 17%




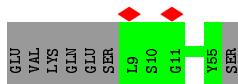
- Molecule 1: Light-harvesting protein B-870 beta chain

Chain O:  81% 19%




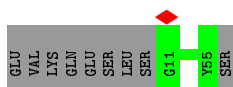
- Molecule 1: Light-harvesting protein B-870 beta chain

Chain Q:  87% 13%




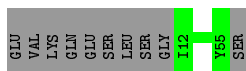
- Molecule 1: Light-harvesting protein B-870 beta chain

Chain S:  83% 17%




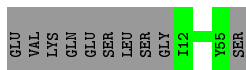
- Molecule 1: Light-harvesting protein B-870 beta chain

Chain U:  81% 19%




- Molecule 1: Light-harvesting protein B-870 beta chain

Chain W:  81% 19%




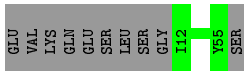
- Molecule 1: Light-harvesting protein B-870 beta chain

Chain Y:  76% 20%




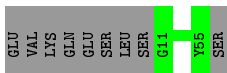
- Molecule 1: Light-harvesting protein B-870 beta chain

Chain d:  81% 19%




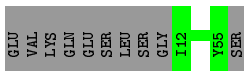
- Molecule 1: Light-harvesting protein B-870 beta chain

Chain m:  83% 17%



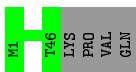
- Molecule 1: Light-harvesting protein B-870 beta chain

Chain n:  81% 19%




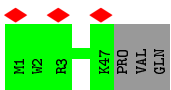
- Molecule 2: Antenna complex, alpha/beta subunit

Chain 2:  92% 8%




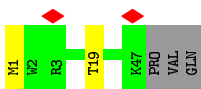
- Molecule 2: Antenna complex, alpha/beta subunit

Chain 4:  94% 6% 6%

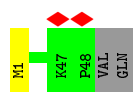


- Molecule 2: Antenna complex, alpha/beta subunit

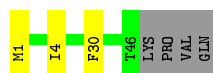
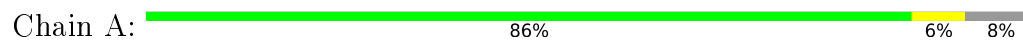
Chain 6:  90% 6%



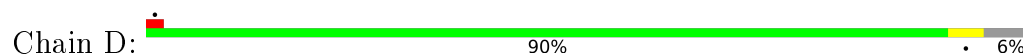
- Molecule 2: Antenna complex, alpha/beta subunit



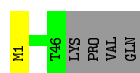
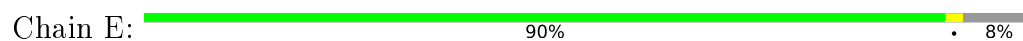
- Molecule 2: Antenna complex, alpha/beta subunit



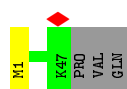
- Molecule 2: Antenna complex, alpha/beta subunit



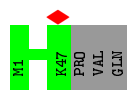
- Molecule 2: Antenna complex, alpha/beta subunit



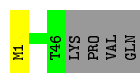
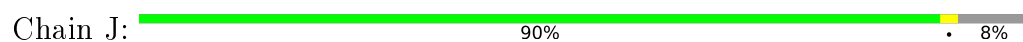
- Molecule 2: Antenna complex, alpha/beta subunit




- Molecule 2: Antenna complex, alpha/beta subunit

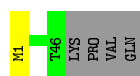


- Molecule 2: Antenna complex, alpha/beta subunit



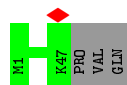
- Molecule 2: Antenna complex, alpha/beta subunit

Chain N:  90% 8%



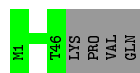
- Molecule 2: Antenna complex, alpha/beta subunit

Chain T:  94% 6%



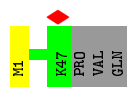
- Molecule 2: Antenna complex, alpha/beta subunit

Chain V:  92% 8%



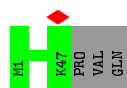
- Molecule 2: Antenna complex, alpha/beta subunit

Chain X:  92% 6%



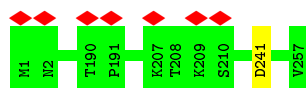
- Molecule 2: Antenna complex, alpha/beta subunit

Chain Z:  94% 6%



- Molecule 3: Photosynthetic reaction center, H-chain

Chain H:  100%



- Molecule 4: Photosynthetic reaction center L subunit

Chain L:  96%



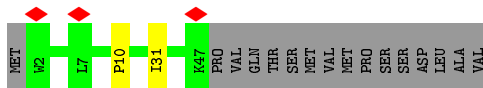
- Molecule 5: Reaction center protein M chain

Chain M: 98%



- Molecule 6: Antenna complex, alpha/beta subunit

Chain R: 5% 71% 26%





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	519005	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	120000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.161	Depositor
Minimum map value	-0.071	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0165	Depositor
Map size ( $\text{\AA}$ )	332.8, 332.8, 332.8	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.3, 1.3, 1.3	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 07D, PO4, FME, U10, CL, RQ0, FE, CD4, LMT, BPH, PGW, CRT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	1	0.26	0/376	0.40	0/514
1	3	0.26	0/376	0.41	0/514
1	5	0.26	0/376	0.43	0/514
1	7	0.26	0/376	0.42	0/514
1	9	0.27	0/386	0.43	0/527
1	I	0.26	0/376	0.41	0/514
1	K	0.26	0/380	0.40	0/519
1	O	0.26	0/376	0.40	0/514
1	Q	0.25	0/394	0.44	0/538
1	S	0.26	0/380	0.42	0/519
1	U	0.26	0/376	0.41	0/514
1	W	0.26	0/376	0.41	0/514
1	Y	0.27	0/368	0.46	0/503
1	d	0.25	0/376	0.41	0/514
1	m	0.26	0/380	0.44	0/519
1	n	0.26	0/376	0.42	0/514
2	2	0.26	0/390	0.54	0/532
2	4	0.26	0/399	0.54	0/543
2	6	0.26	0/399	0.56	0/543
2	8	0.25	0/407	0.55	0/555
2	A	0.26	0/390	0.54	0/532
2	D	0.25	0/399	0.52	0/543
2	E	0.26	0/390	0.54	0/532
2	F	0.26	0/399	0.53	0/543
2	G	0.26	0/399	0.51	0/543
2	J	0.25	0/390	0.52	0/532
2	N	0.26	0/390	0.54	0/532
2	T	0.26	0/399	0.54	0/543
2	V	0.26	0/390	0.53	0/532
2	X	0.26	0/399	0.53	0/543
2	Z	0.26	0/399	0.54	0/543
3	H	0.25	0/2014	0.59	0/2739

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
4	L	0.25	0/2248	0.51	0/3077
5	M	0.26	0/2515	0.52	0/3429
6	R	0.26	0/399	0.55	0/543
All	All	0.26	0/19163	0.50	0/26144

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [\(i\)](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	360	0	350	0	0
1	3	360	0	350	0	0
1	5	360	0	350	0	0
1	7	360	0	350	1	0
1	9	370	0	358	0	0
1	I	360	0	350	1	0
1	K	364	0	353	0	0
1	O	360	0	350	0	0
1	Q	378	0	369	0	0
1	S	364	0	353	0	0
1	U	360	0	350	0	0
1	W	360	0	350	0	0
1	Y	352	0	339	2	0
1	d	360	0	350	0	0
1	m	364	0	353	0	0
1	n	360	0	350	0	0
2	2	388	0	394	0	0
2	4	397	0	407	0	0
2	6	397	0	407	2	0
2	8	404	0	414	0	0
2	A	388	0	394	2	0
2	D	397	0	407	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	388	0	394	0	0
2	F	397	0	407	0	0
2	G	397	0	407	0	0
2	J	388	0	394	0	0
2	N	388	0	394	0	0
2	T	397	0	407	0	0
2	V	388	0	394	0	0
2	X	397	0	407	0	0
2	Z	397	0	407	0	0
3	H	1972	0	2023	0	0
4	L	2164	0	2126	4	0
5	M	2424	0	2365	3	0
6	R	387	0	396	2	0
7	1	66	0	0	0	0
7	2	66	0	0	0	0
7	3	66	0	0	0	0
7	4	66	0	0	0	0
7	5	66	0	0	0	0
7	6	66	0	0	0	0
7	7	66	0	0	0	0
7	8	66	0	0	0	0
7	9	66	0	0	0	0
7	A	66	0	0	0	0
7	D	66	0	0	0	0
7	E	66	0	0	0	0
7	F	66	0	0	0	0
7	G	66	0	0	0	0
7	H	66	0	0	0	0
7	I	66	0	0	0	0
7	J	66	0	0	0	0
7	K	66	0	0	0	0
7	L	132	0	0	0	0
7	M	132	0	0	0	0
7	N	66	0	0	0	0
7	O	66	0	0	0	0
7	Q	66	0	0	0	0
7	R	66	0	0	0	0
7	S	66	0	0	0	0
7	T	66	0	0	0	0
7	U	66	0	0	0	0
7	V	66	0	0	0	0
7	W	66	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	X	66	0	0	0	0
7	Y	66	0	0	0	0
7	Z	66	0	0	0	0
7	d	66	0	0	0	0
7	m	66	0	0	0	0
7	n	66	0	0	0	0
8	1	44	0	60	0	0
8	3	44	0	60	0	0
8	5	44	0	60	3	0
8	7	44	0	60	0	0
8	9	44	0	60	0	0
8	I	44	0	60	1	0
8	J	44	0	60	1	0
8	K	44	0	60	0	0
8	M	44	0	60	2	0
8	N	44	0	60	1	0
8	O	44	0	60	0	0
8	Q	44	0	60	0	0
8	S	44	0	60	0	0
8	Y	44	0	60	1	0
8	d	44	0	60	0	0
8	m	44	0	60	0	0
8	n	44	0	60	0	0
9	H	102	0	152	0	0
10	H	84	0	124	0	0
10	M	84	0	124	0	0
11	L	65	0	76	1	0
11	M	65	0	76	1	0
12	L	62	0	0	0	0
13	L	126	0	180	3	0
13	M	63	0	90	1	0
14	M	1	0	0	0	0
15	M	1	0	0	0	0
16	M	5	0	0	0	0
17	R	35	0	45	0	0
18	2	1	0	0	0	0
18	3	1	0	0	0	0
18	4	11	0	0	0	0
18	5	2	0	0	0	0
18	6	8	0	0	0	0
18	7	1	0	0	0	0
18	8	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	9	1	0	0	0	0
18	A	8	0	0	0	0
18	D	6	0	0	0	0
18	E	5	0	0	0	0
18	F	6	0	0	0	0
18	G	8	0	0	0	0
18	H	68	0	0	0	0
18	I	1	0	0	0	0
18	J	3	0	0	0	0
18	K	1	0	0	0	0
18	L	89	0	0	0	0
18	M	86	0	0	0	0
18	N	14	0	0	0	0
18	O	3	0	0	0	0
18	Q	2	0	0	0	0
18	R	8	0	0	0	0
18	S	2	0	0	0	0
18	T	4	0	0	0	0
18	U	3	0	0	0	0
18	V	4	0	0	0	0
18	W	1	0	0	0	0
18	X	8	0	0	0	0
18	Y	1	0	0	0	0
18	Z	7	0	0	0	0
18	d	2	0	0	0	0
18	n	1	0	0	0	0
All	All	22902	0	20456	23	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

The worst 5 of 23 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:1006:U10:H3M3	6:R:31:ILE:HA	1.84	0.59
4:L:133:VAL:HG23	4:L:134:VAL:HG23	1.91	0.52
2:6:19:THR:HG23	5:M:58:LEU:HD23	1.92	0.52
4:L:174:HIS:CE1	4:L:178:ILE:HD11	2.44	0.51
4:L:44:VAL:HG21	13:M:403:U10:H551	1.93	0.50

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	42/54 (78%)	41 (98%)	1 (2%)	0	100	100
1	3	42/54 (78%)	41 (98%)	1 (2%)	0	100	100
1	5	42/54 (78%)	42 (100%)	0	0	100	100
1	7	42/54 (78%)	41 (98%)	1 (2%)	0	100	100
1	9	44/54 (82%)	44 (100%)	0	0	100	100
1	I	42/54 (78%)	41 (98%)	1 (2%)	0	100	100
1	K	43/54 (80%)	42 (98%)	1 (2%)	0	100	100
1	O	42/54 (78%)	41 (98%)	1 (2%)	0	100	100
1	Q	45/54 (83%)	45 (100%)	0	0	100	100
1	S	43/54 (80%)	43 (100%)	0	0	100	100
1	U	42/54 (78%)	41 (98%)	1 (2%)	0	100	100
1	W	42/54 (78%)	42 (100%)	0	0	100	100
1	Y	41/54 (76%)	40 (98%)	1 (2%)	0	100	100
1	d	42/54 (78%)	42 (100%)	0	0	100	100
1	m	43/54 (80%)	42 (98%)	1 (2%)	0	100	100
1	n	42/54 (78%)	42 (100%)	0	0	100	100
2	2	44/50 (88%)	44 (100%)	0	0	100	100
2	4	45/50 (90%)	43 (96%)	2 (4%)	0	100	100
2	6	45/50 (90%)	43 (96%)	2 (4%)	0	100	100
2	8	46/50 (92%)	45 (98%)	1 (2%)	0	100	100
2	A	44/50 (88%)	44 (100%)	0	0	100	100
2	D	45/50 (90%)	44 (98%)	1 (2%)	0	100	100
2	E	44/50 (88%)	43 (98%)	1 (2%)	0	100	100
2	F	45/50 (90%)	45 (100%)	0	0	100	100
2	G	45/50 (90%)	43 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	44/50 (88%)	43 (98%)	1 (2%)	0	100	100
2	N	44/50 (88%)	43 (98%)	1 (2%)	0	100	100
2	T	45/50 (90%)	44 (98%)	1 (2%)	0	100	100
2	V	44/50 (88%)	43 (98%)	1 (2%)	0	100	100
2	X	45/50 (90%)	45 (100%)	0	0	100	100
2	Z	45/50 (90%)	44 (98%)	1 (2%)	0	100	100
3	H	255/257 (99%)	246 (96%)	9 (4%)	0	100	100
4	L	272/276 (99%)	264 (97%)	8 (3%)	0	100	100
5	M	303/306 (99%)	292 (96%)	11 (4%)	0	100	100
6	R	44/62 (71%)	43 (98%)	1 (2%)	0	100	100
All	All	2223/2515 (88%)	2171 (98%)	52 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	36/45 (80%)	36 (100%)	0	100	100
1	3	36/45 (80%)	36 (100%)	0	100	100
1	5	36/45 (80%)	36 (100%)	0	100	100
1	7	36/45 (80%)	36 (100%)	0	100	100
1	9	37/45 (82%)	37 (100%)	0	100	100
1	I	36/45 (80%)	36 (100%)	0	100	100
1	K	36/45 (80%)	36 (100%)	0	100	100
1	O	36/45 (80%)	36 (100%)	0	100	100
1	Q	38/45 (84%)	38 (100%)	0	100	100
1	S	36/45 (80%)	36 (100%)	0	100	100
1	U	36/45 (80%)	36 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	W	36/45 (80%)	36 (100%)	0	100	100
1	Y	35/45 (78%)	35 (100%)	0	100	100
1	d	36/45 (80%)	36 (100%)	0	100	100
1	m	36/45 (80%)	36 (100%)	0	100	100
1	n	36/45 (80%)	36 (100%)	0	100	100
2	2	39/43 (91%)	39 (100%)	0	100	100
2	4	40/43 (93%)	40 (100%)	0	100	100
2	6	40/43 (93%)	40 (100%)	0	100	100
2	8	41/43 (95%)	41 (100%)	0	100	100
2	A	39/43 (91%)	39 (100%)	0	100	100
2	D	40/43 (93%)	40 (100%)	0	100	100
2	E	39/43 (91%)	39 (100%)	0	100	100
2	F	40/43 (93%)	40 (100%)	0	100	100
2	G	40/43 (93%)	40 (100%)	0	100	100
2	J	39/43 (91%)	39 (100%)	0	100	100
2	N	39/43 (91%)	39 (100%)	0	100	100
2	T	40/43 (93%)	40 (100%)	0	100	100
2	V	39/43 (91%)	39 (100%)	0	100	100
2	X	40/43 (93%)	40 (100%)	0	100	100
2	Z	40/43 (93%)	40 (100%)	0	100	100
3	H	204/204 (100%)	203 (100%)	1 (0%)	88	96
4	L	219/220 (100%)	217 (99%)	2 (1%)	78	92
5	M	239/240 (100%)	237 (99%)	2 (1%)	81	93
6	R	40/55 (73%)	40 (100%)	0	100	100
All	All	1875/2084 (90%)	1870 (100%)	5 (0%)	92	97

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	H	241	ASP
4	L	248	CYS
4	L	273	TRP
5	M	195	PHE
5	M	215	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	H	216	GLN
2	T	12	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

15 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	FME	6	1	2	8,9,10	0.95	0	7,9,11	0.93	0
2	FME	A	1	2	8,9,10	0.88	0	7,9,11	1.13	1 (14%)
2	FME	2	1	2	8,9,10	0.92	0	7,9,11	1.01	0
2	FME	Z	1	2	8,9,10	0.94	0	7,9,11	0.88	0
2	FME	N	1	2	8,9,10	0.91	0	7,9,11	1.06	1 (14%)
2	FME	E	1	2	8,9,10	0.94	0	7,9,11	1.12	1 (14%)
2	FME	V	1	2	8,9,10	0.93	0	7,9,11	1.02	0
2	FME	X	1	2	8,9,10	0.94	0	7,9,11	1.08	1 (14%)
2	FME	4	1	2	8,9,10	0.91	0	7,9,11	0.89	0
2	FME	T	1	2	8,9,10	0.92	0	7,9,11	1.02	0
2	FME	D	1	2	8,9,10	0.91	0	7,9,11	1.09	1 (14%)
2	FME	J	1	2	8,9,10	0.91	0	7,9,11	1.18	1 (14%)
2	FME	8	1	2	8,9,10	0.92	0	7,9,11	1.06	1 (14%)
2	FME	F	1	2	8,9,10	0.90	0	7,9,11	1.13	1 (14%)
2	FME	G	1	2	8,9,10	0.94	0	7,9,11	1.10	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FME	6	1	2	-	1/7/9/11	-
2	FME	A	1	2	-	1/7/9/11	-
2	FME	2	1	2	-	0/7/9/11	-
2	FME	Z	1	2	-	0/7/9/11	-
2	FME	N	1	2	-	0/7/9/11	-
2	FME	E	1	2	-	2/7/9/11	-
2	FME	V	1	2	-	1/7/9/11	-
2	FME	X	1	2	-	2/7/9/11	-
2	FME	4	1	2	-	1/7/9/11	-
2	FME	T	1	2	-	1/7/9/11	-
2	FME	D	1	2	-	1/7/9/11	-
2	FME	J	1	2	-	1/7/9/11	-
2	FME	8	1	2	-	3/7/9/11	-
2	FME	F	1	2	-	1/7/9/11	-
2	FME	G	1	2	-	3/7/9/11	-

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	1	FME	C-CA-N	2.57	114.38	109.73
2	E	1	FME	C-CA-N	2.46	114.16	109.73
2	X	1	FME	C-CA-N	2.38	114.03	109.73
2	F	1	FME	C-CA-N	2.37	114.00	109.73
2	A	1	FME	C-CA-N	2.23	113.77	109.73

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	8	1	FME	O-C-CA-CB
2	D	1	FME	O-C-CA-CB
2	G	1	FME	CB-CA-N-CN
2	G	1	FME	O-C-CA-CB
2	J	1	FME	C-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	6	1	FME	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 68 ligands modelled in this entry, 2 are monoatomic - leaving 66 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
8	CRT	M	406	-	41,43,43	0.54	0	50,54,54	0.85	1 (2%)
7	07D	3	102	-	65,74,74	1.95	10 (15%)	65,115,115	3.26	15 (23%)
7	07D	X	1001	-	65,74,74	1.94	10 (15%)	65,115,115	3.18	15 (23%)
8	CRT	N	1001	-	41,43,43	0.60	0	50,54,54	0.88	2 (4%)
8	CRT	n	101	-	41,43,43	0.58	0	50,54,54	0.85	1 (2%)
7	07D	Q	102	-	65,74,74	1.94	10 (15%)	65,115,115	3.21	14 (21%)
7	07D	4	1001	-	65,74,74	1.94	10 (15%)	65,115,115	3.20	15 (23%)
7	07D	W	1001	-	65,74,74	1.94	10 (15%)	65,115,115	3.23	15 (23%)
8	CRT	3	101	-	41,43,43	0.63	0	50,54,54	0.69	0
7	07D	I	102	-	65,74,74	1.94	10 (15%)	65,115,115	3.24	14 (21%)
7	07D	T	101	-	65,74,74	1.94	10 (15%)	65,115,115	3.23	15 (23%)
7	07D	n	102	-	65,74,74	1.94	10 (15%)	65,115,115	3.28	14 (21%)
7	07D	L	1005	-	65,74,74	1.98	10 (15%)	65,115,115	3.24	14 (21%)
8	CRT	K	101	-	41,43,43	0.57	0	50,54,54	0.75	0
8	CRT	1	1002	-	41,43,43	0.62	0	50,54,54	0.85	0
8	CRT	O	101	-	41,43,43	0.59	0	50,54,54	0.69	0
13	U10	L	1006	-	63,63,63	0.16	0	76,79,79	0.68	1 (1%)
13	U10	L	1003	-	63,63,63	0.19	0	76,79,79	0.46	0
17	LMT	R	102	-	36,36,36	1.10	5 (13%)	47,47,47	0.84	2 (4%)
8	CRT	d	1001	-	41,43,43	0.64	0	50,54,54	1.02	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	CRT	I	101	-	41,43,43	0.57	0	50,54,54	0.76	0
7	07D	6	1001	-	65,74,74	1.94	10 (15%)	65,115,115	3.17	15 (23%)
7	07D	7	102	-	65,74,74	1.94	10 (15%)	65,115,115	3.28	13 (20%)
7	07D	M	404	-	65,74,74	2.00	11 (16%)	65,115,115	3.16	15 (23%)
7	07D	U	1001	-	65,74,74	1.94	10 (15%)	65,115,115	3.22	14 (21%)
7	07D	2	1001	-	65,74,74	1.96	10 (15%)	65,115,115	3.10	15 (23%)
13	U10	M	403	-	63,63,63	0.15	0	76,79,79	0.54	0
7	07D	Z	1001	-	65,74,74	1.95	10 (15%)	65,115,115	3.11	15 (23%)
16	PO4	M	409	-	4,4,4	0.98	0	6,6,6	0.45	0
9	PGW	H	303	7	50,50,50	0.45	0	53,56,56	0.82	2 (3%)
7	07D	R	101	-	65,74,74	1.94	10 (15%)	65,115,115	3.12	16 (24%)
7	07D	1	1001	-	65,74,74	1.94	10 (15%)	65,115,115	3.26	14 (21%)
8	CRT	J	1002	-	41,43,43	0.57	0	50,54,54	0.76	0
7	07D	O	102	-	65,74,74	1.94	10 (15%)	65,115,115	3.23	14 (21%)
7	07D	F	1001	-	65,74,74	1.94	9 (13%)	65,115,115	3.19	15 (23%)
7	07D	J	1001	-	65,74,74	1.94	10 (15%)	65,115,115	3.22	15 (23%)
7	07D	N	1002	-	65,74,74	1.95	10 (15%)	65,115,115	3.17	15 (23%)
8	CRT	9	101	-	41,43,43	0.63	0	50,54,54	1.13	5 (10%)
7	07D	9	102	-	65,74,74	1.93	10 (15%)	65,115,115	3.28	14 (21%)
8	CRT	S	101	-	41,43,43	0.57	0	50,54,54	0.76	0
7	07D	H	301	9	65,74,74	1.96	10 (15%)	65,115,115	3.04	14 (21%)
7	07D	L	1004	-	65,74,74	1.96	10 (15%)	65,115,115	3.23	15 (23%)
7	07D	K	102	-	65,74,74	1.94	10 (15%)	65,115,115	3.25	14 (21%)
7	07D	E	1001	-	65,74,74	1.94	10 (15%)	65,115,115	3.23	15 (23%)
9	PGW	H	302	-	50,50,50	0.47	0	53,56,56	0.92	3 (5%)
10	CD4	H	304	-	83,83,83	0.48	0	89,95,95	0.88	2 (2%)
8	CRT	Q	101	-	41,43,43	0.58	0	50,54,54	0.78	0
7	07D	d	1002	-	65,74,74	1.95	10 (15%)	65,115,115	3.28	14 (21%)
7	07D	m	102	-	65,74,74	1.97	11 (16%)	65,115,115	3.31	15 (23%)
7	07D	M	405	-	65,74,74	1.99	11 (16%)	65,115,115	3.08	16 (24%)
8	CRT	7	101	-	41,43,43	0.59	0	50,54,54	0.74	0
7	07D	S	102	-	65,74,74	1.94	10 (15%)	65,115,115	3.28	15 (23%)
10	CD4	M	407	-	83,83,83	0.47	0	89,95,95	0.89	3 (3%)
7	07D	Y	102	-	65,74,74	1.94	10 (15%)	65,115,115	3.27	16 (24%)
8	CRT	5	101	-	41,43,43	0.60	0	50,54,54	0.74	0
7	07D	A	101	-	65,74,74	1.95	9 (13%)	65,115,115	3.22	15 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	CRT	m	101	-	41,43,43	0.60	0	50,54,54	0.78	0
12	RQ0	L	1002	-	62,62,62	1.58	7 (11%)	69,78,78	1.31	5 (7%)
11	BPH	L	1001	-	64,70,70	0.85	3 (4%)	76,101,101	1.10	6 (7%)
8	CRT	Y	101	-	41,43,43	0.62	0	50,54,54	0.92	1 (2%)
11	BPH	M	402	-	64,70,70	0.85	3 (4%)	76,101,101	1.17	6 (7%)
7	07D	8	1001	-	65,74,74	1.96	10 (15%)	65,115,115	3.08	15 (23%)
7	07D	G	1001	-	65,74,74	1.96	10 (15%)	65,115,115	3.08	14 (21%)
7	07D	V	1001	-	65,74,74	1.94	10 (15%)	65,115,115	3.21	14 (21%)
7	07D	D	1001	-	65,74,74	1.94	9 (13%)	65,115,115	3.16	15 (23%)
7	07D	5	102	-	65,74,74	1.93	10 (15%)	65,115,115	3.26	14 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	CRT	M	406	-	-	8/51/51/51	-
7	07D	3	102	-	1/1/21/28	8/41/137/137	-
7	07D	X	1001	-	1/1/21/28	10/41/137/137	-
8	CRT	N	1001	-	-	4/51/51/51	-
8	CRT	n	101	-	-	2/51/51/51	-
7	07D	Q	102	-	1/1/21/28	5/41/137/137	-
7	07D	4	1001	-	1/1/21/28	7/41/137/137	-
7	07D	W	1001	-	1/1/21/28	6/41/137/137	-
8	CRT	3	101	-	-	6/51/51/51	-
7	07D	I	102	-	1/1/21/28	4/41/137/137	-
7	07D	T	101	-	1/1/21/28	6/41/137/137	-
7	07D	n	102	-	1/1/21/28	11/41/137/137	-
7	07D	L	1005	-	1/1/21/28	10/41/137/137	-
8	CRT	K	101	-	-	3/51/51/51	-
8	CRT	1	1002	-	-	4/51/51/51	-
8	CRT	O	101	-	-	7/51/51/51	-
13	U10	L	1006	-	-	7/63/87/87	0/1/1/1
13	U10	L	1003	-	-	10/63/87/87	0/1/1/1
17	LMT	R	102	-	-	2/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	CRT	d	1001	-	-	2/51/51/51	-
8	CRT	I	101	-	-	2/51/51/51	-
7	07D	6	1001	-	1/1/21/28	8/41/137/137	-
7	07D	7	102	-	1/1/21/28	8/41/137/137	-
7	07D	M	404	-	1/1/21/28	8/41/137/137	-
7	07D	U	1001	-	1/1/21/28	4/41/137/137	-
7	07D	2	1001	-	1/1/21/28	6/41/137/137	-
13	U10	M	403	-	-	8/63/87/87	0/1/1/1
7	07D	Z	1001	-	1/1/21/28	7/41/137/137	-
9	PGW	H	303	7	-	8/55/55/55	-
7	07D	R	101	-	1/1/21/28	10/41/137/137	-
7	07D	1	1001	-	1/1/21/28	6/41/137/137	-
8	CRT	J	1002	-	-	0/51/51/51	-
7	07D	O	102	-	1/1/21/28	5/41/137/137	-
7	07D	F	1001	-	1/1/21/28	12/41/137/137	-
7	07D	J	1001	-	1/1/21/28	6/41/137/137	-
7	07D	N	1002	-	1/1/21/28	5/41/137/137	-
8	CRT	9	101	-	-	6/51/51/51	-
7	07D	9	102	-	1/1/21/28	4/41/137/137	-
8	CRT	S	101	-	-	4/51/51/51	-
7	07D	H	301	9	1/1/21/28	15/41/137/137	-
7	07D	L	1004	-	1/1/21/28	7/41/137/137	-
7	07D	K	102	-	1/1/21/28	3/41/137/137	-
7	07D	E	1001	-	1/1/21/28	8/41/137/137	-
9	PGW	H	302	-	-	13/55/55/55	-
10	CD4	H	304	-	-	11/94/94/94	-
8	CRT	Q	101	-	-	2/51/51/51	-
7	07D	d	1002	-	1/1/21/28	11/41/137/137	-
7	07D	m	102	-	1/1/21/28	5/41/137/137	-
7	07D	M	405	-	1/1/21/28	6/41/137/137	-
8	CRT	7	101	-	-	2/51/51/51	-
7	07D	S	102	-	1/1/21/28	4/41/137/137	-
10	CD4	M	407	-	-	14/94/94/94	-
7	07D	Y	102	-	1/1/21/28	7/41/137/137	-

*Continued on next page...*

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	CRT	5	101	-	-	4/51/51/51	-
7	07D	A	101	-	1/1/21/28	9/41/137/137	-
8	CRT	m	101	-	-	3/51/51/51	-
12	RQ0	L	1002	-	-	18/61/85/85	0/1/1/1
11	BPH	L	1001	-	-	5/54/105/105	0/5/6/6
8	CRT	Y	101	-	-	1/51/51/51	-
11	BPH	M	402	-	-	4/54/105/105	0/5/6/6
7	07D	8	1001	-	1/1/21/28	7/41/137/137	-
7	07D	G	1001	-	1/1/21/28	7/41/137/137	-
7	07D	V	1001	-	1/1/21/28	10/41/137/137	-
7	07D	D	1001	-	1/1/21/28	6/41/137/137	-
7	07D	5	102	-	1/1/21/28	10/41/137/137	-

The worst 5 of 388 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	1002	RQ0	C11-C07	7.68	1.54	1.34
12	L	1002	RQ0	C18-C14	7.64	1.54	1.34
7	M	404	07D	C1C-NC	-6.38	1.29	1.35
7	L	1005	07D	C1C-NC	-6.34	1.29	1.35
7	d	1002	07D	C1C-NC	-6.26	1.29	1.35

The worst 5 of 586 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	m	102	07D	CAA-C2A-C1A	-16.84	109.18	127.48
7	9	102	07D	CAA-C2A-C1A	-16.80	109.23	127.48
7	d	1002	07D	CAA-C2A-C1A	-16.51	109.54	127.48
7	S	102	07D	CAA-C2A-C1A	-16.39	109.67	127.48
7	Y	102	07D	CAA-C2A-C1A	-16.33	109.73	127.48

5 of 37 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	1	1001	07D	NA
7	2	1001	07D	NA
7	3	102	07D	NA
7	4	1001	07D	NA
7	5	102	07D	NA



5 of 431 torsion outliers are listed below:

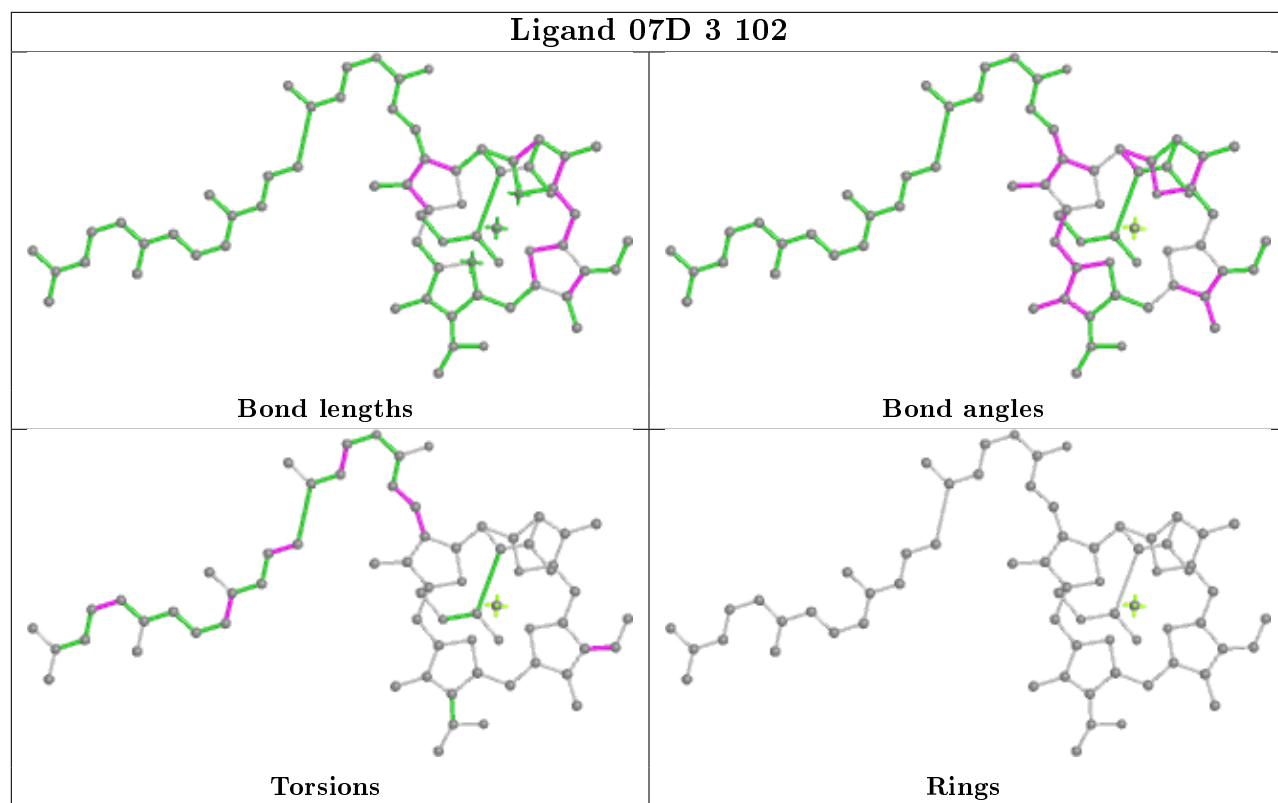
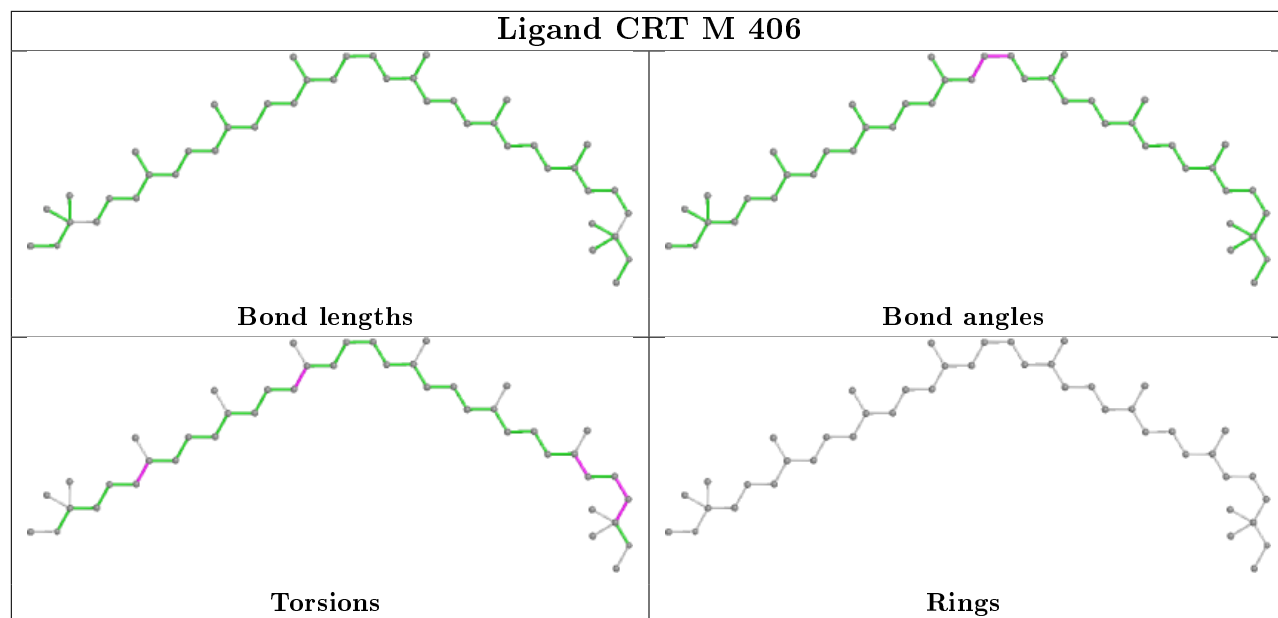
Mol	Chain	Res	Type	Atoms
7	1	1001	07D	C1A-C2A-CAA-CBA
7	1	1001	07D	C4C-C3C-CAC-CBC
7	2	1001	07D	C3-C5-C6-C7
7	2	1001	07D	C8-C10-C11-C12
7	2	1001	07D	C4C-C3C-CAC-CBC

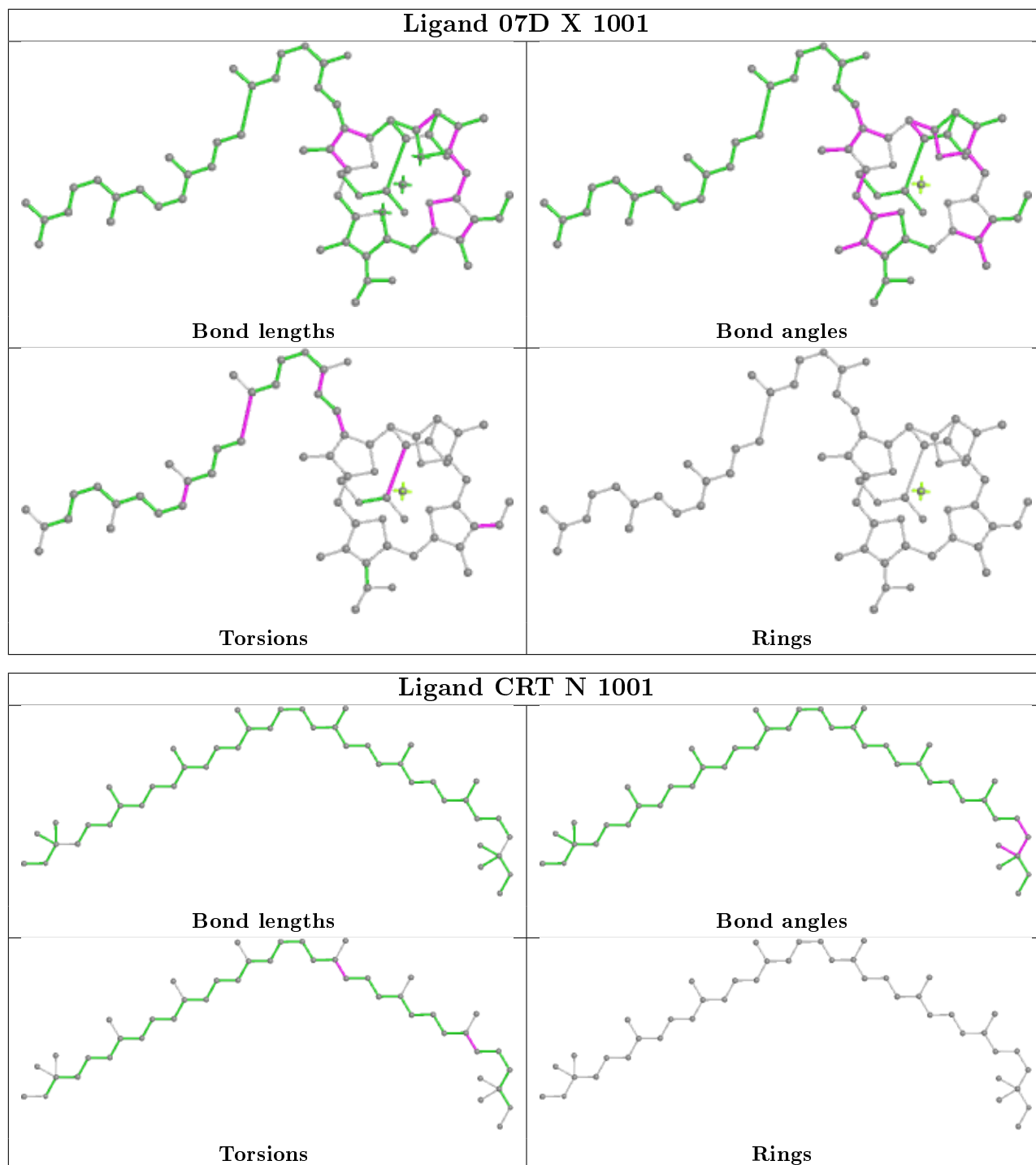
There are no ring outliers.

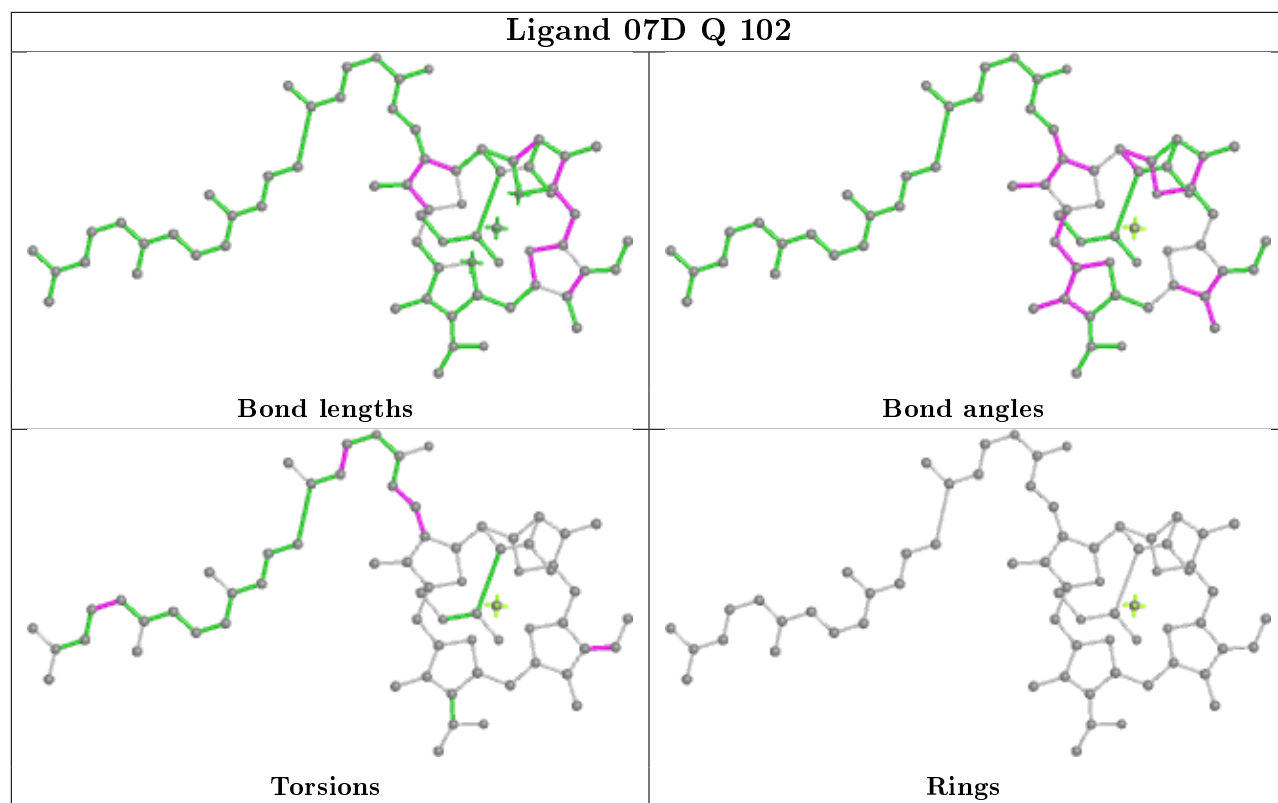
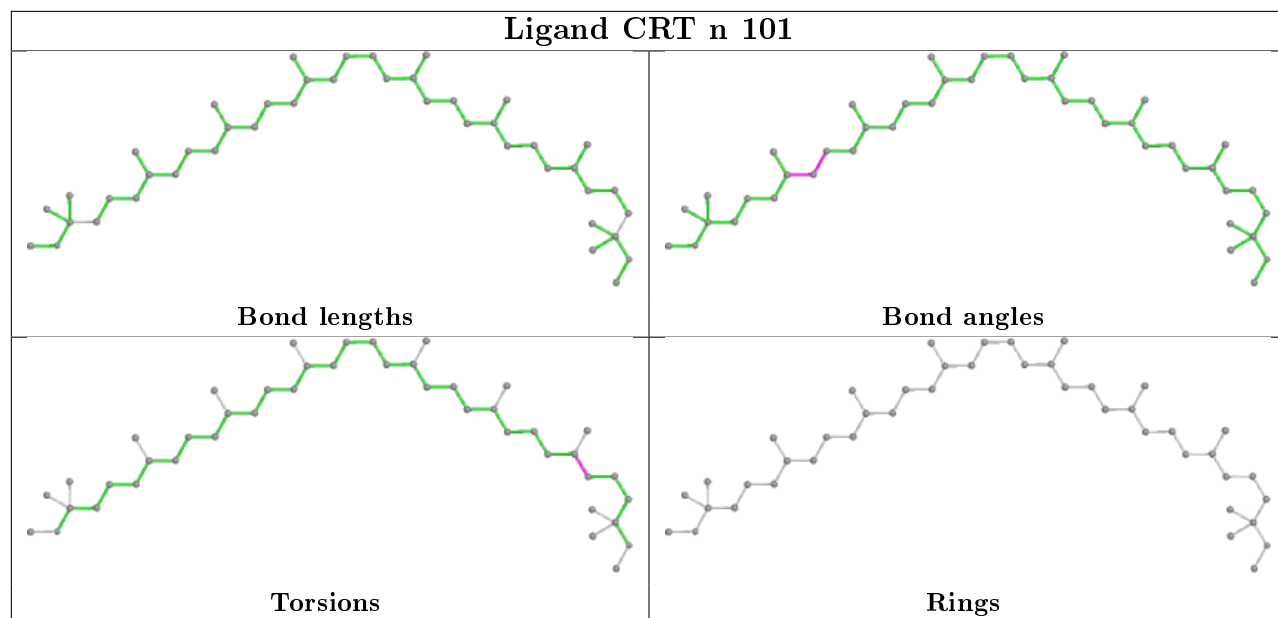
10 monomers are involved in 15 short contacts:

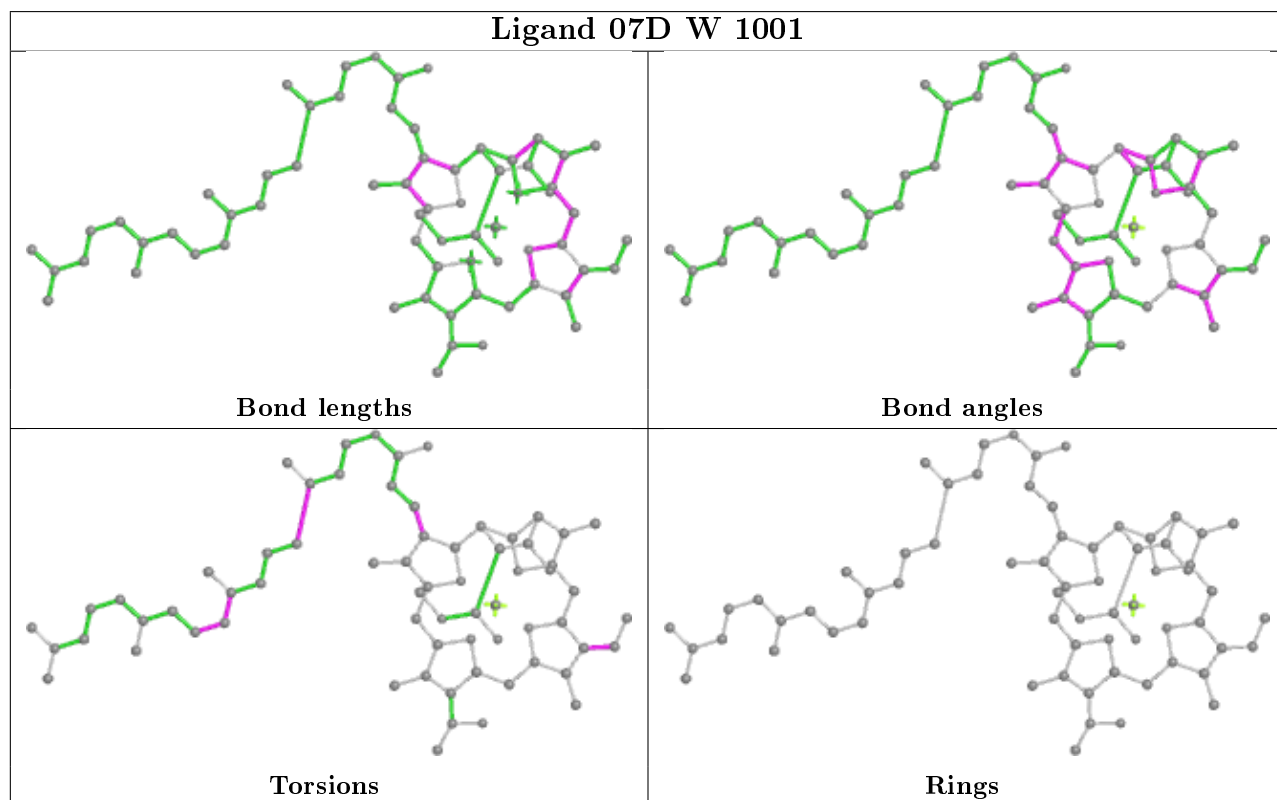
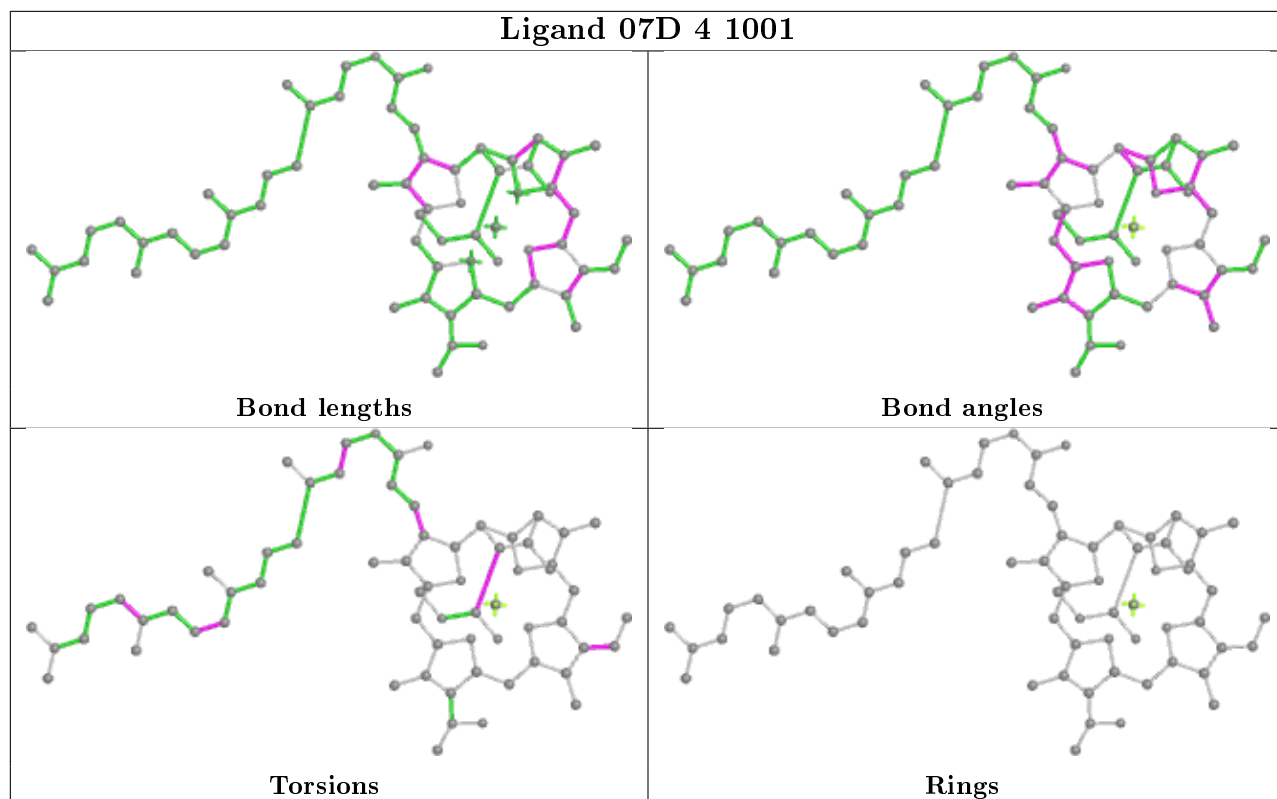
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	M	406	CRT	2	0
8	N	1001	CRT	1	0
13	L	1006	U10	3	0
8	I	101	CRT	1	0
13	M	403	U10	1	0
8	J	1002	CRT	1	0
8	5	101	CRT	3	0
11	L	1001	BPH	1	0
8	Y	101	CRT	1	0
11	M	402	BPH	1	0

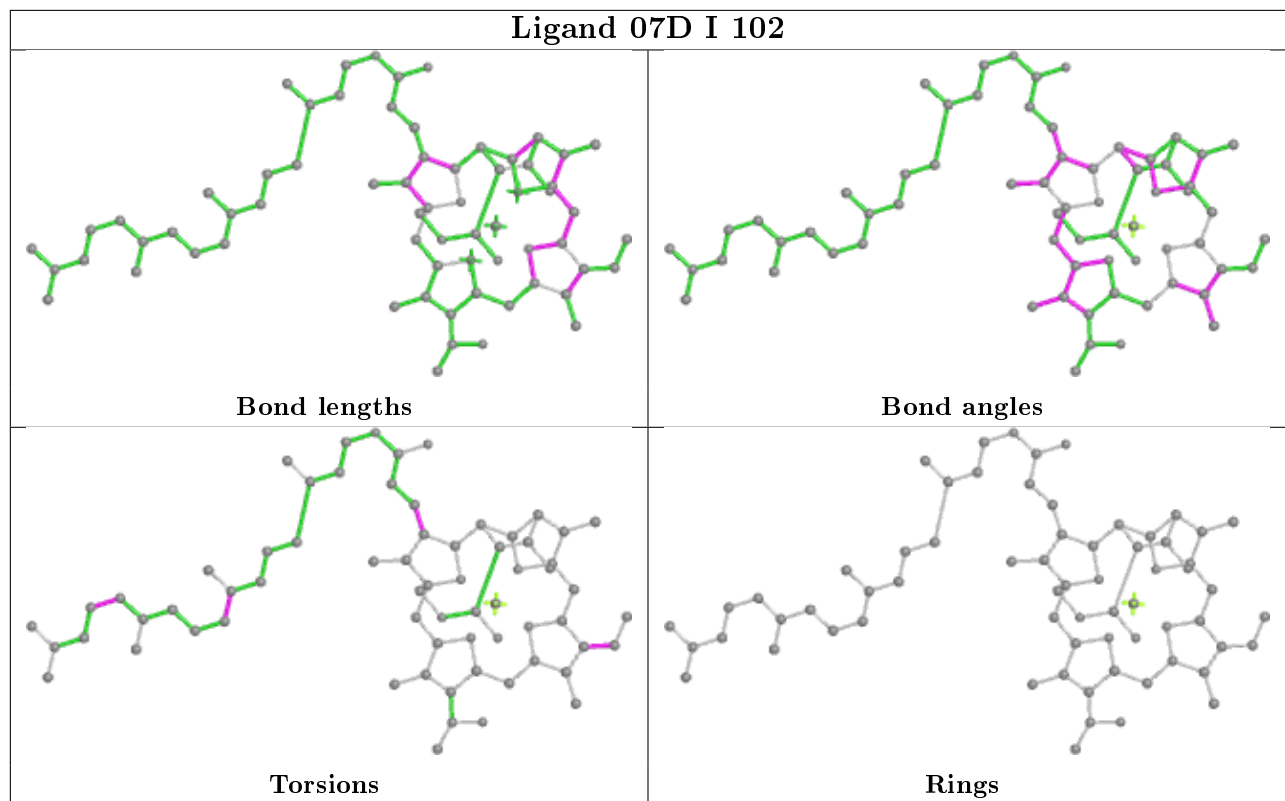
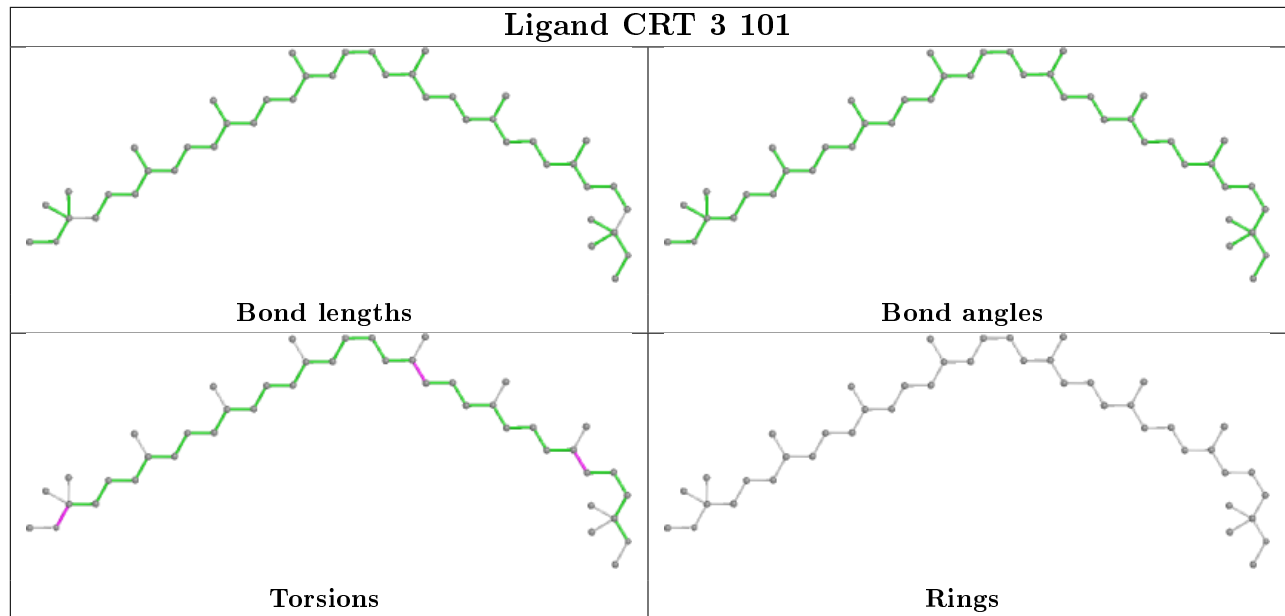
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

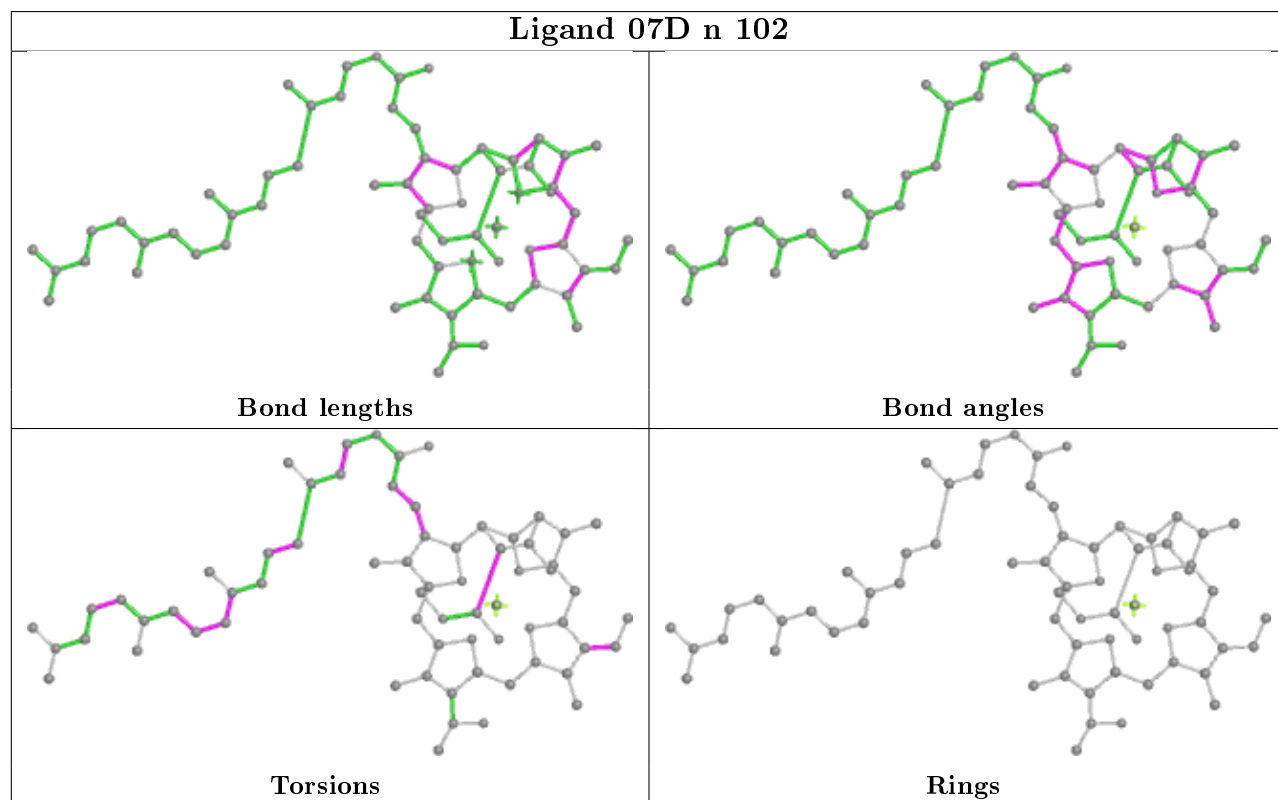
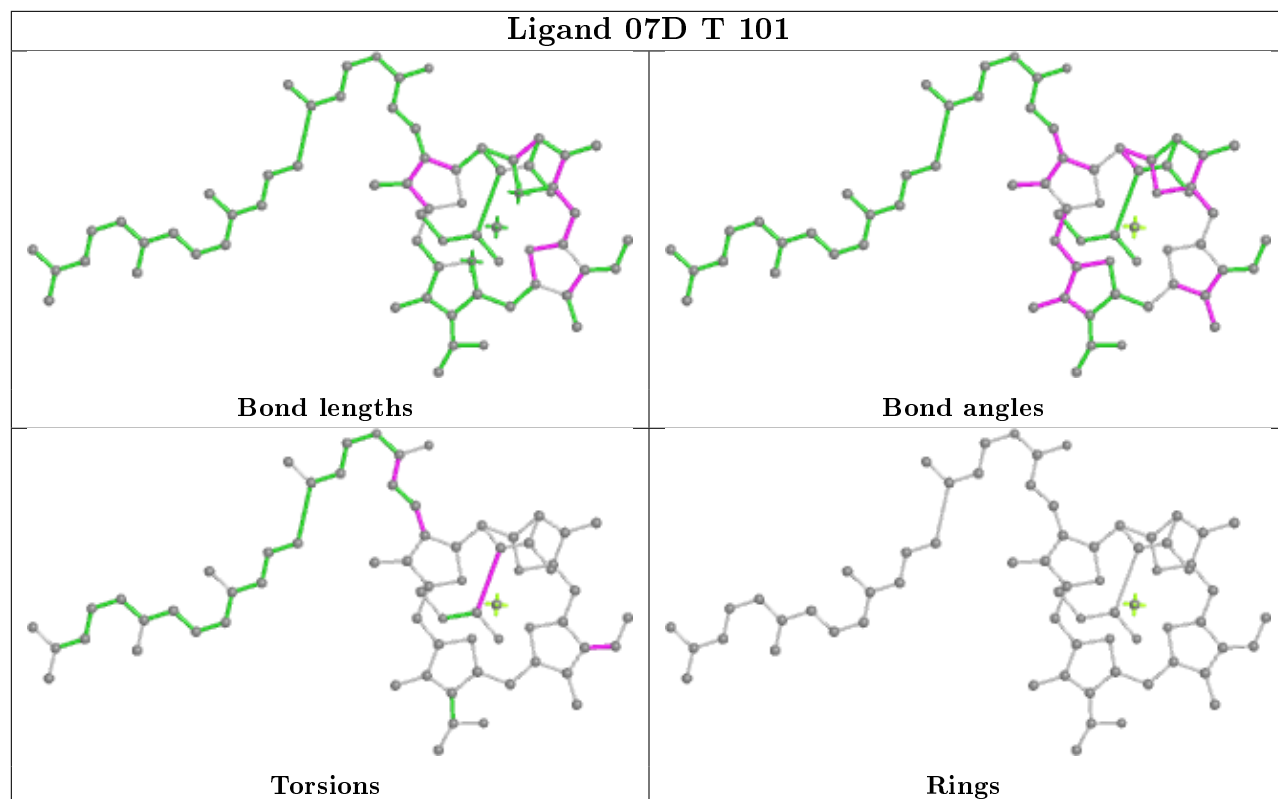


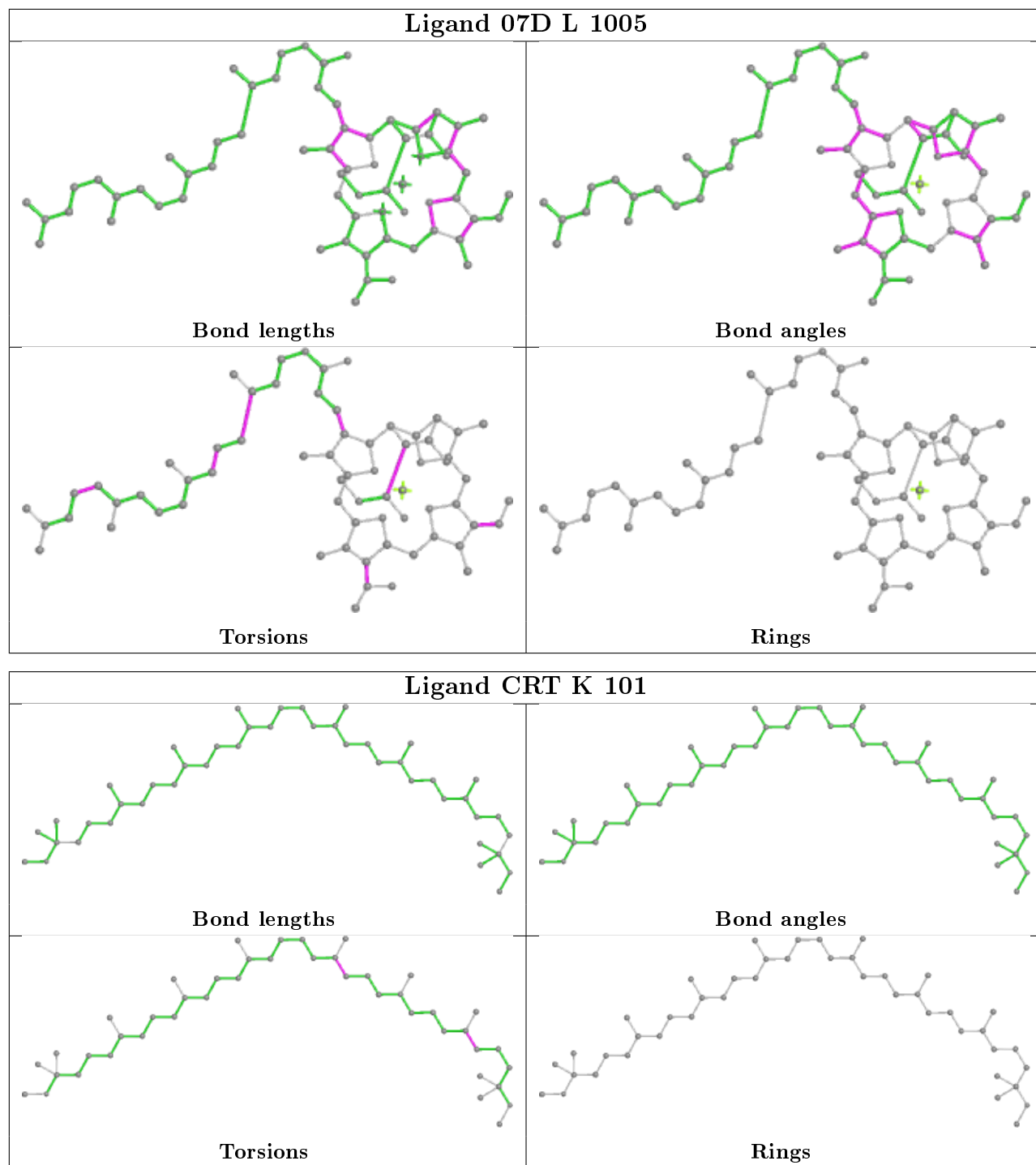




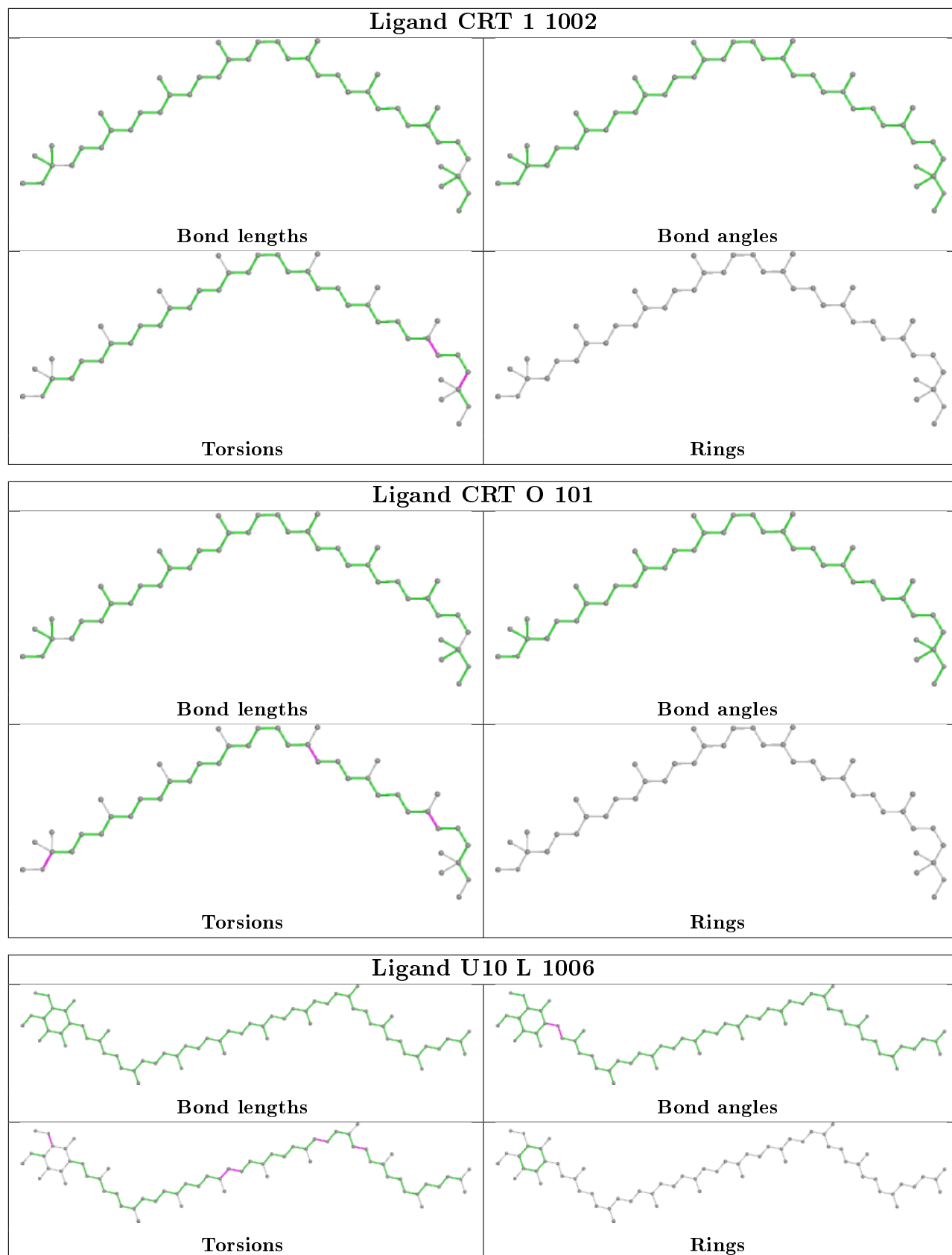


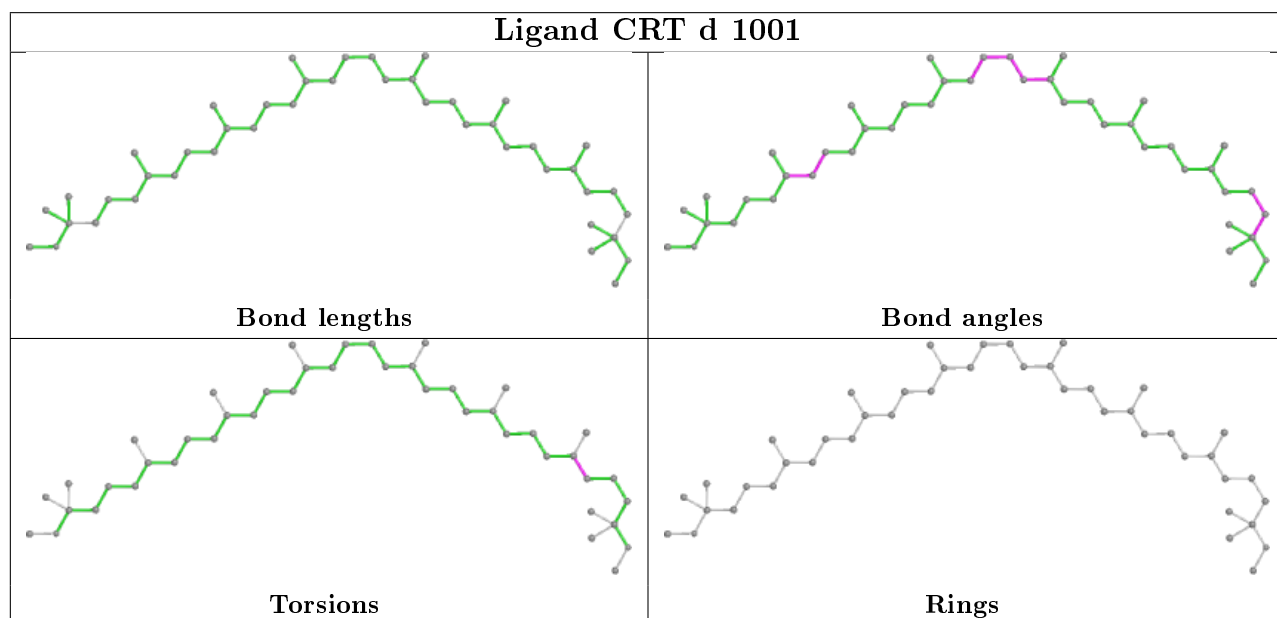
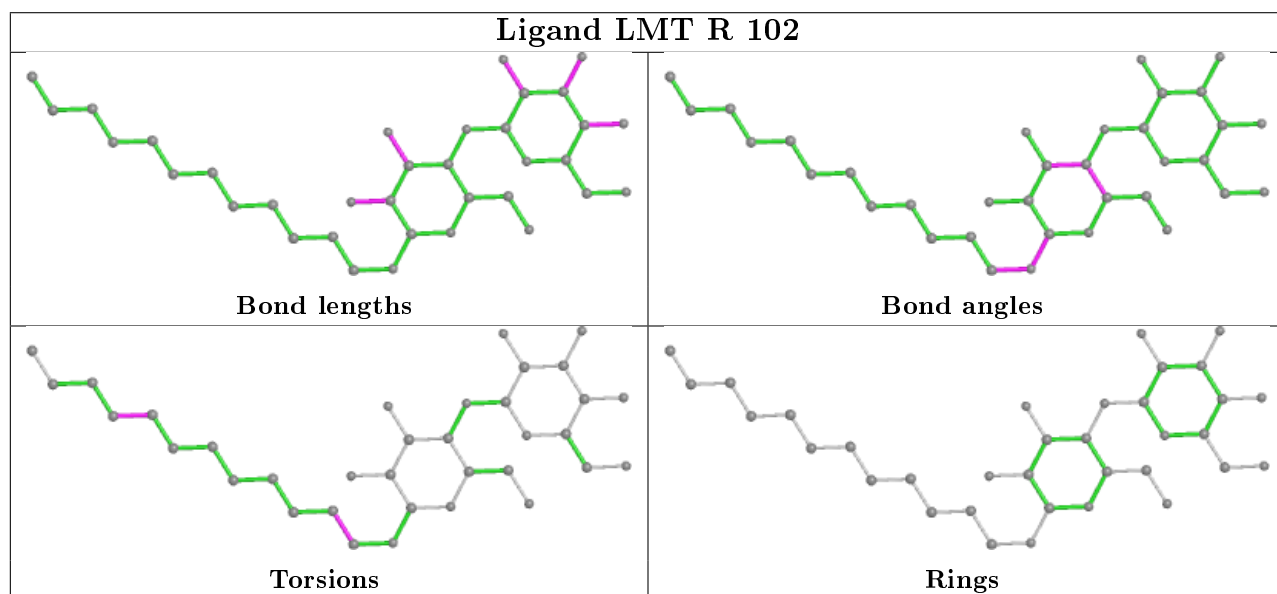
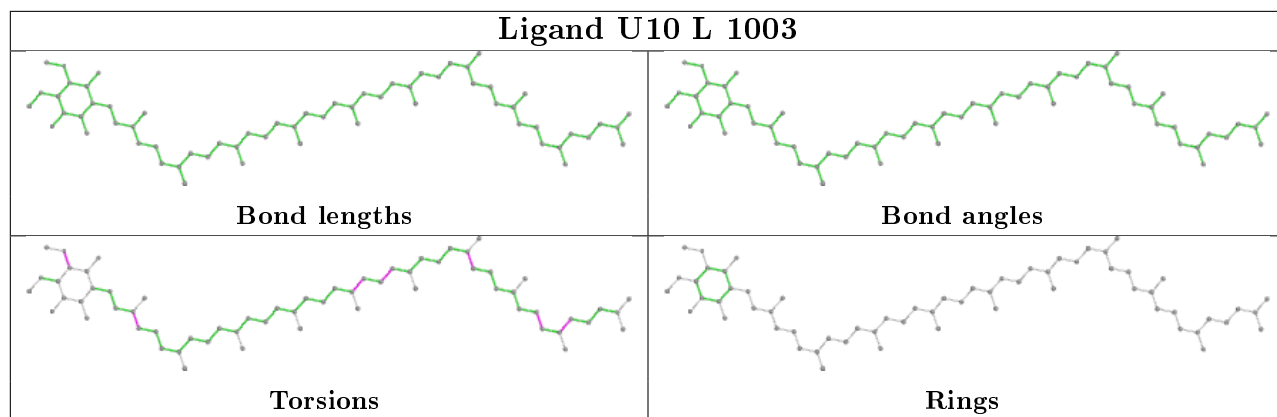


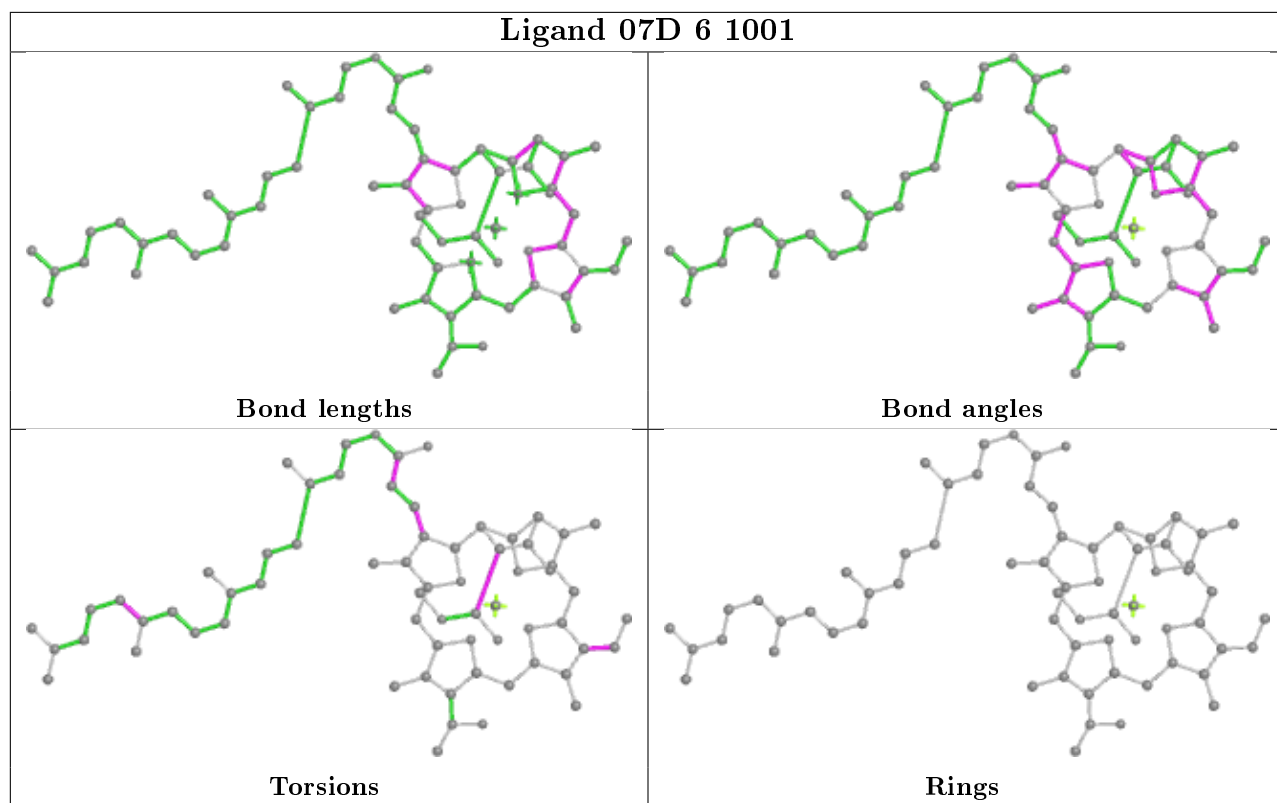
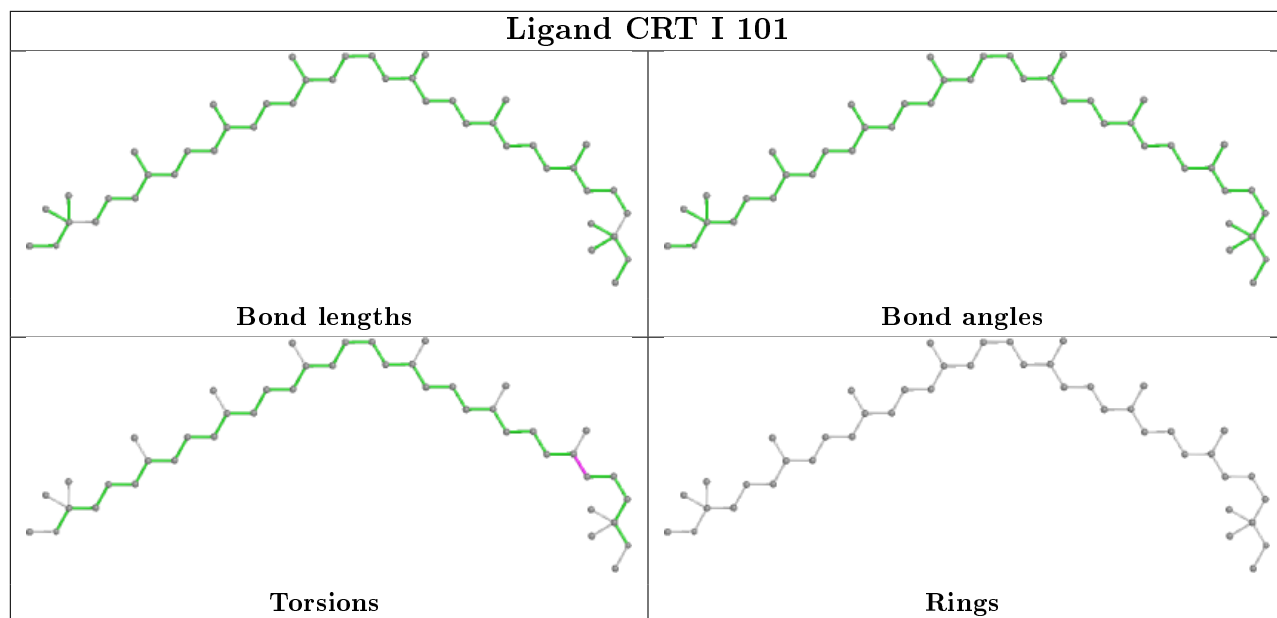


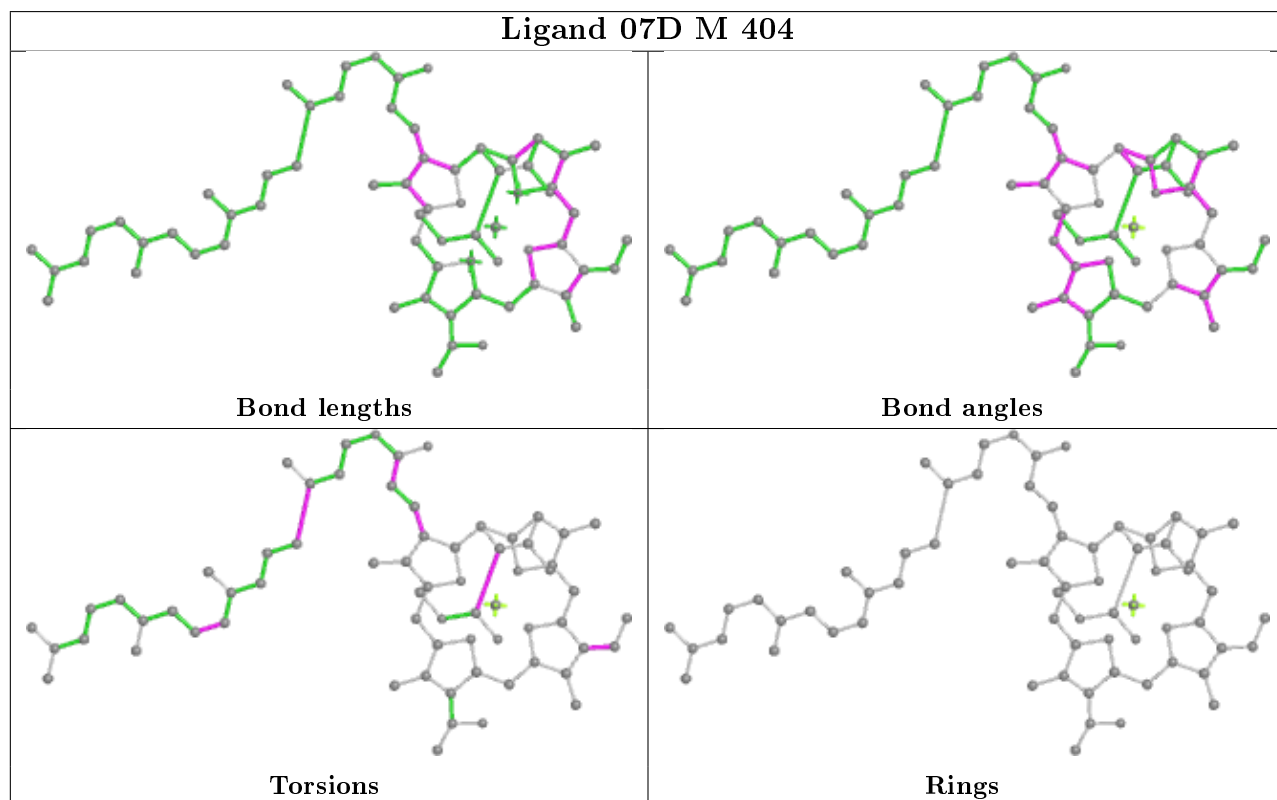
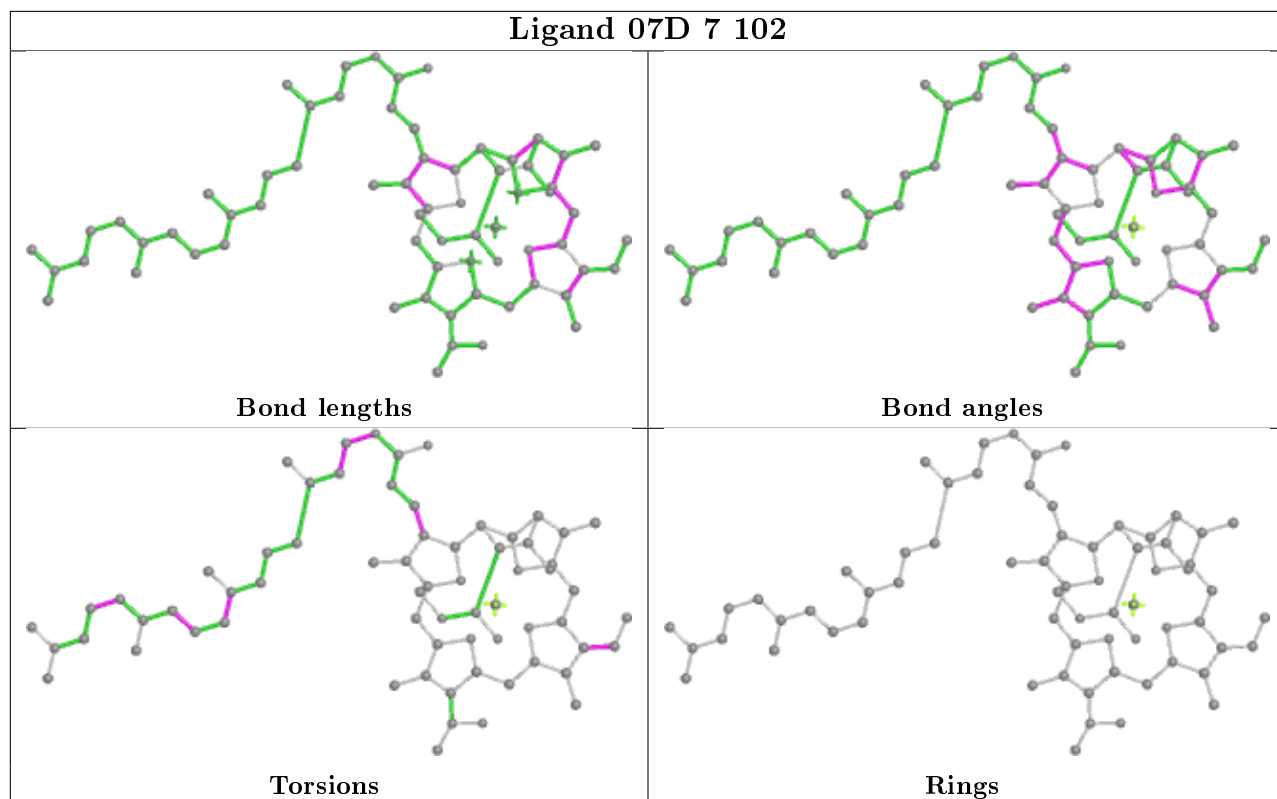


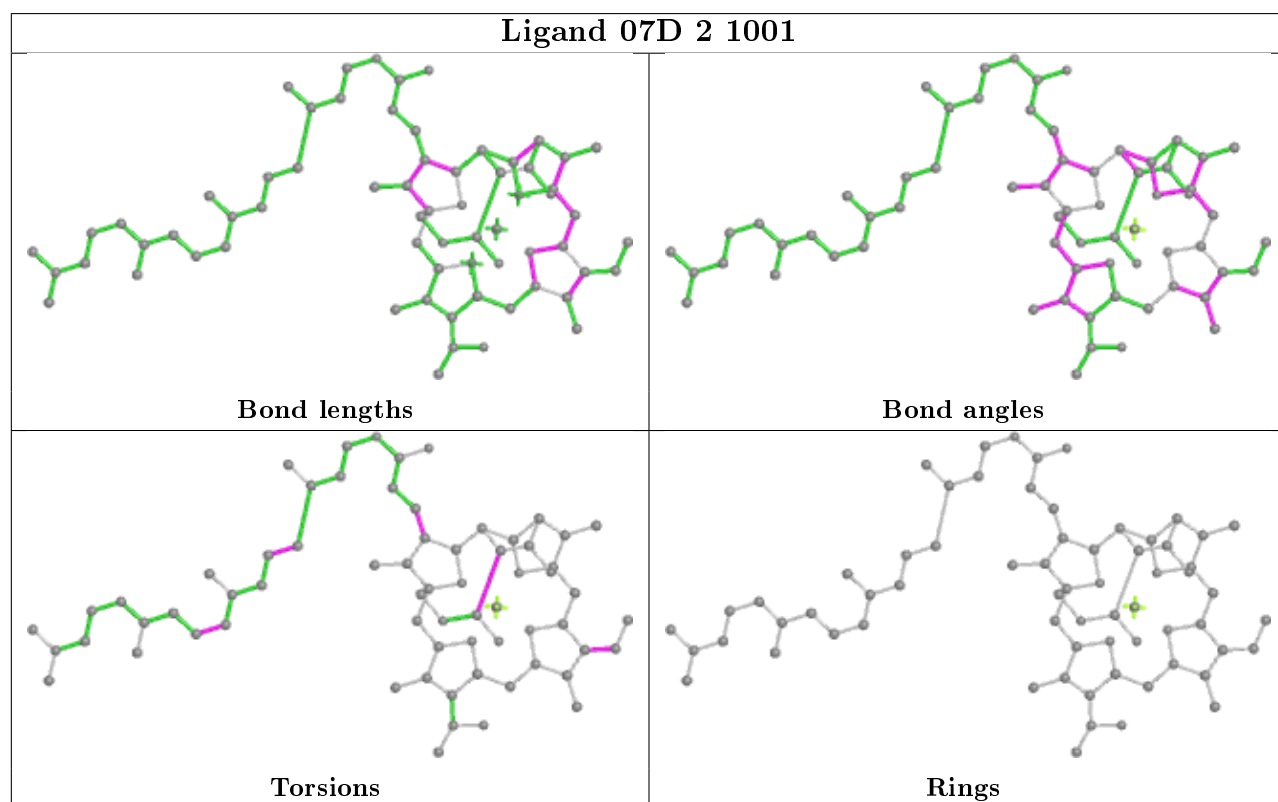
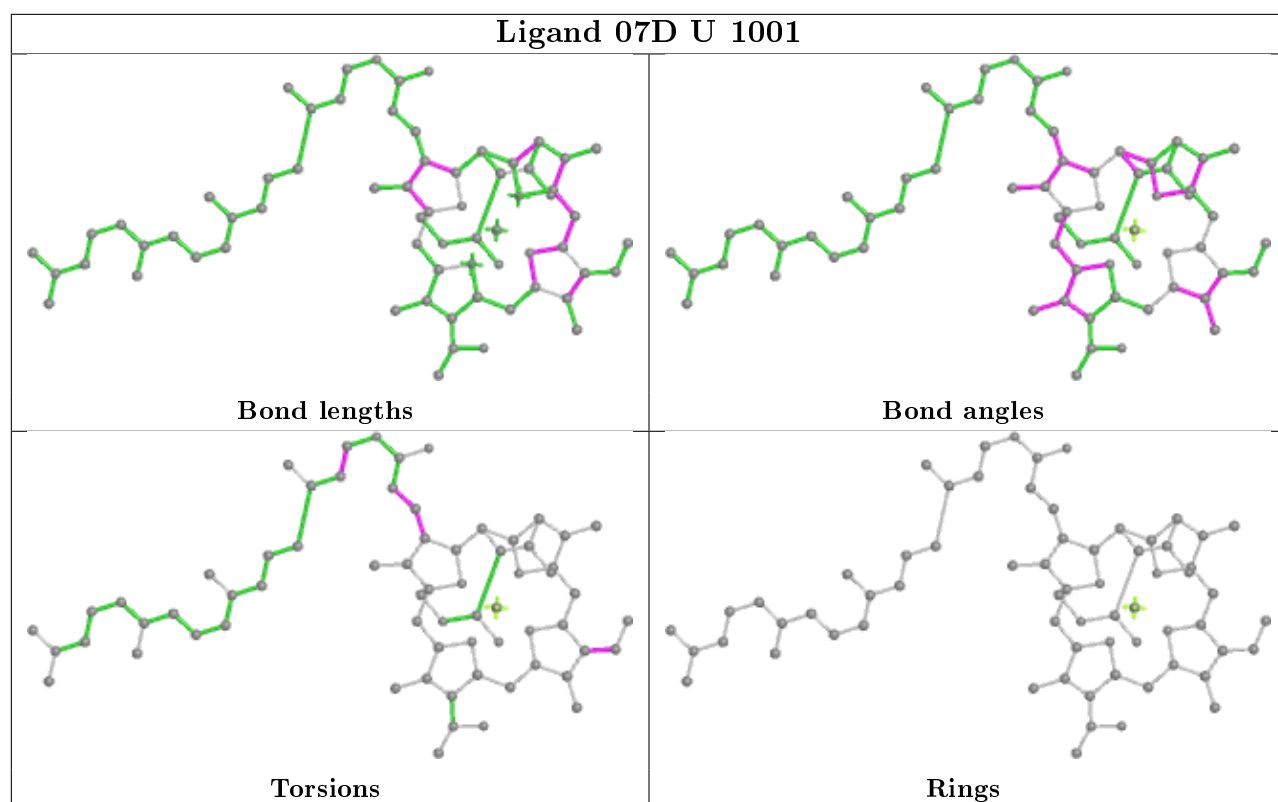


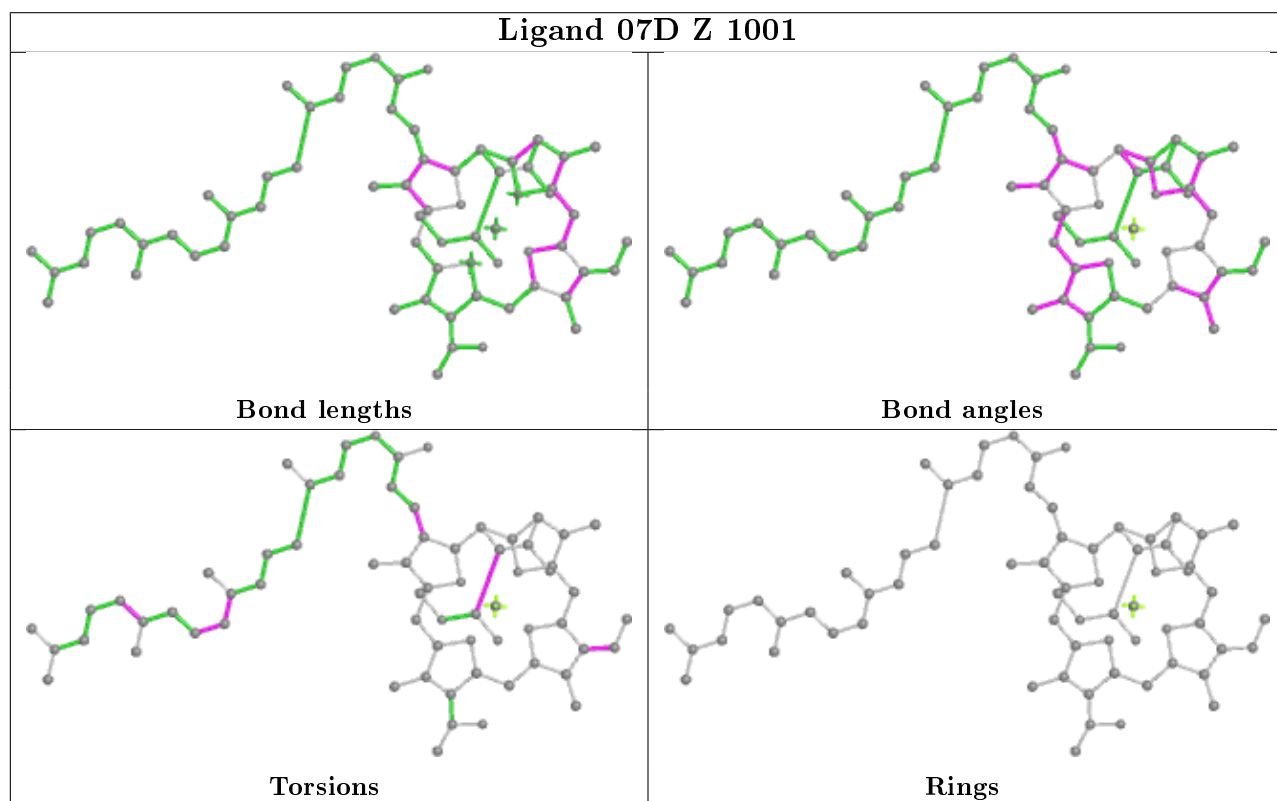
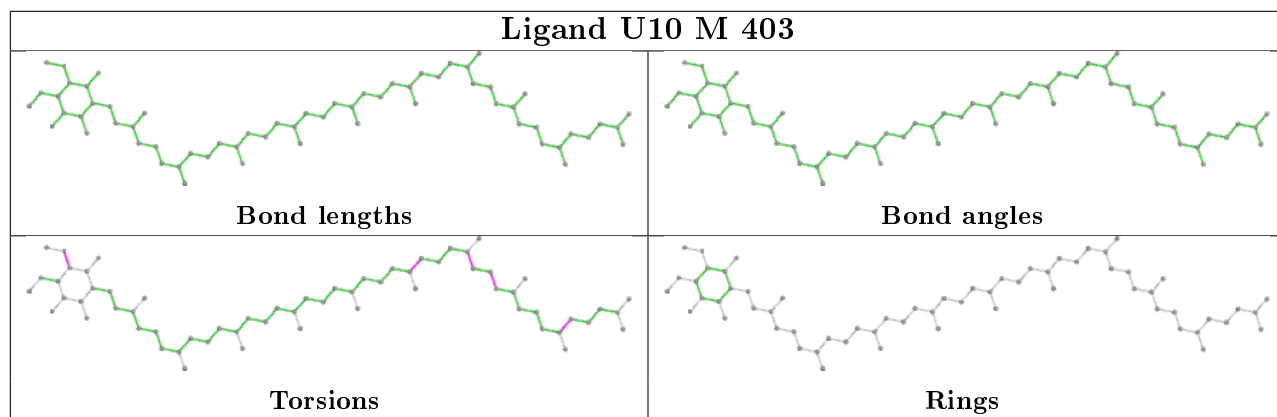


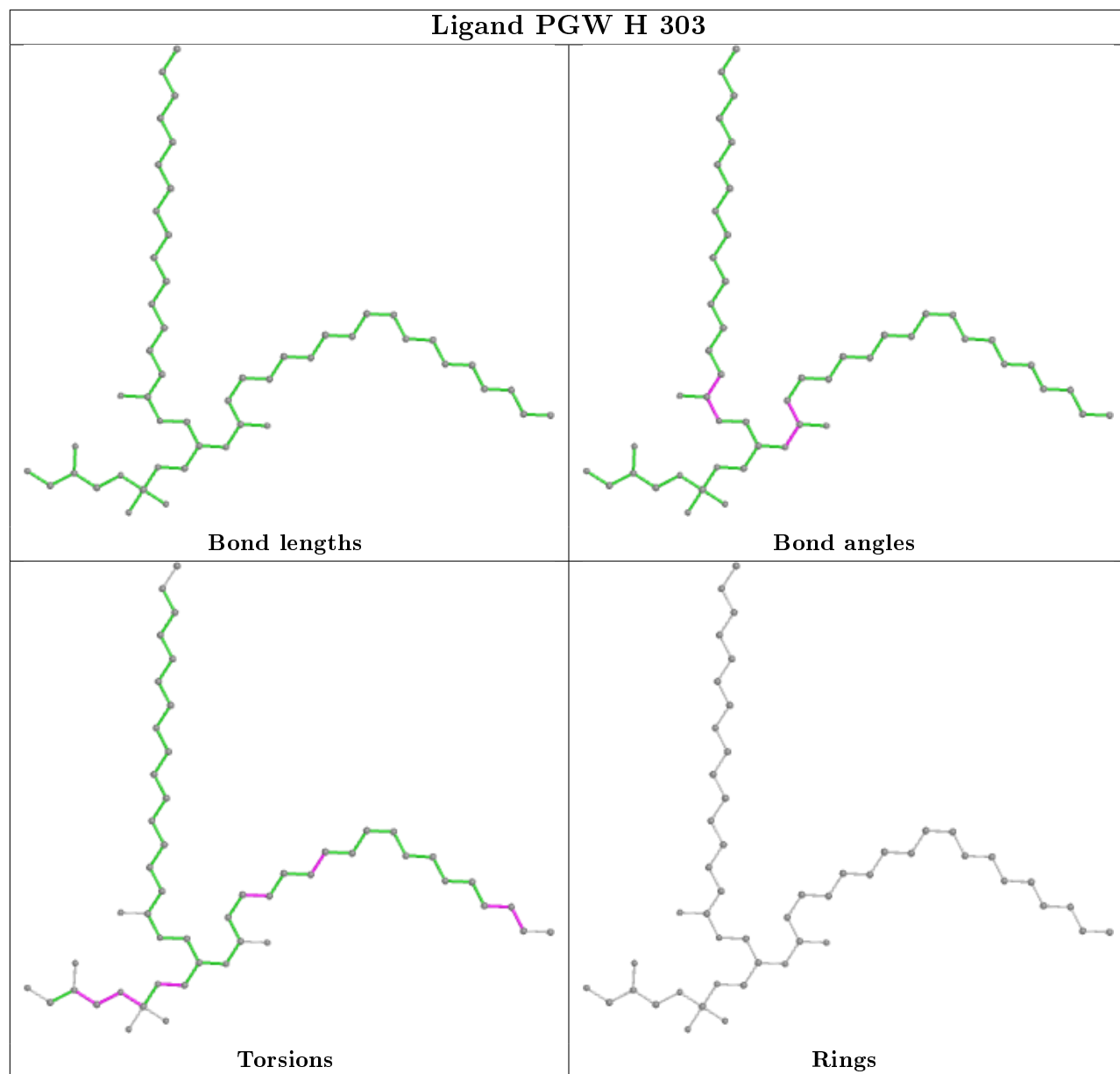


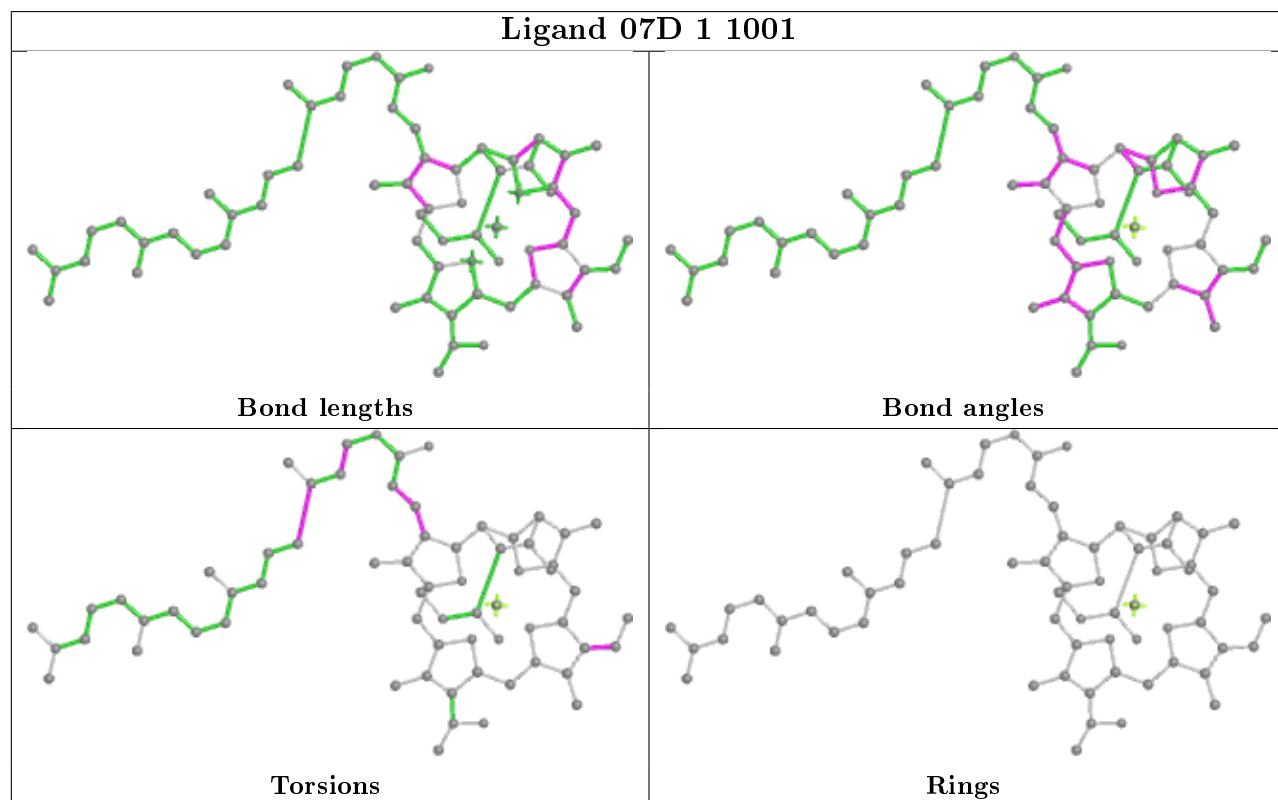
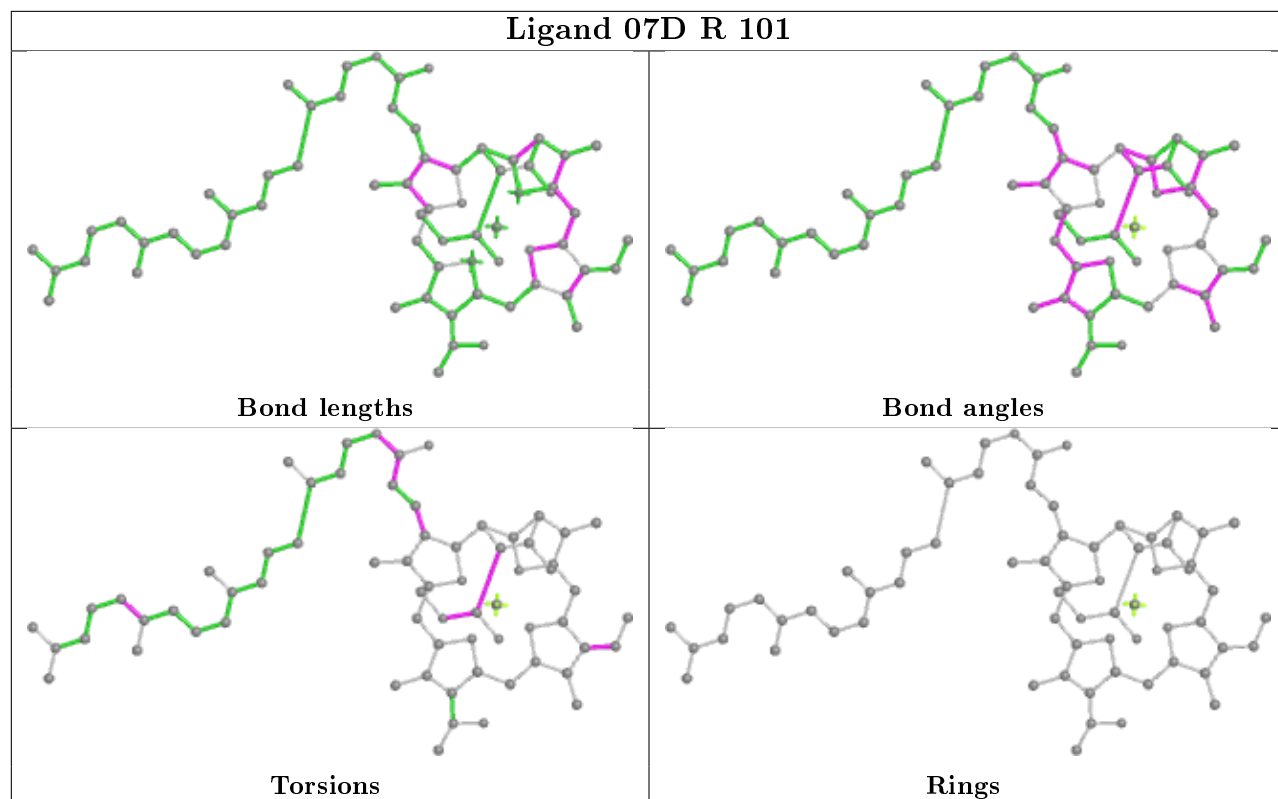




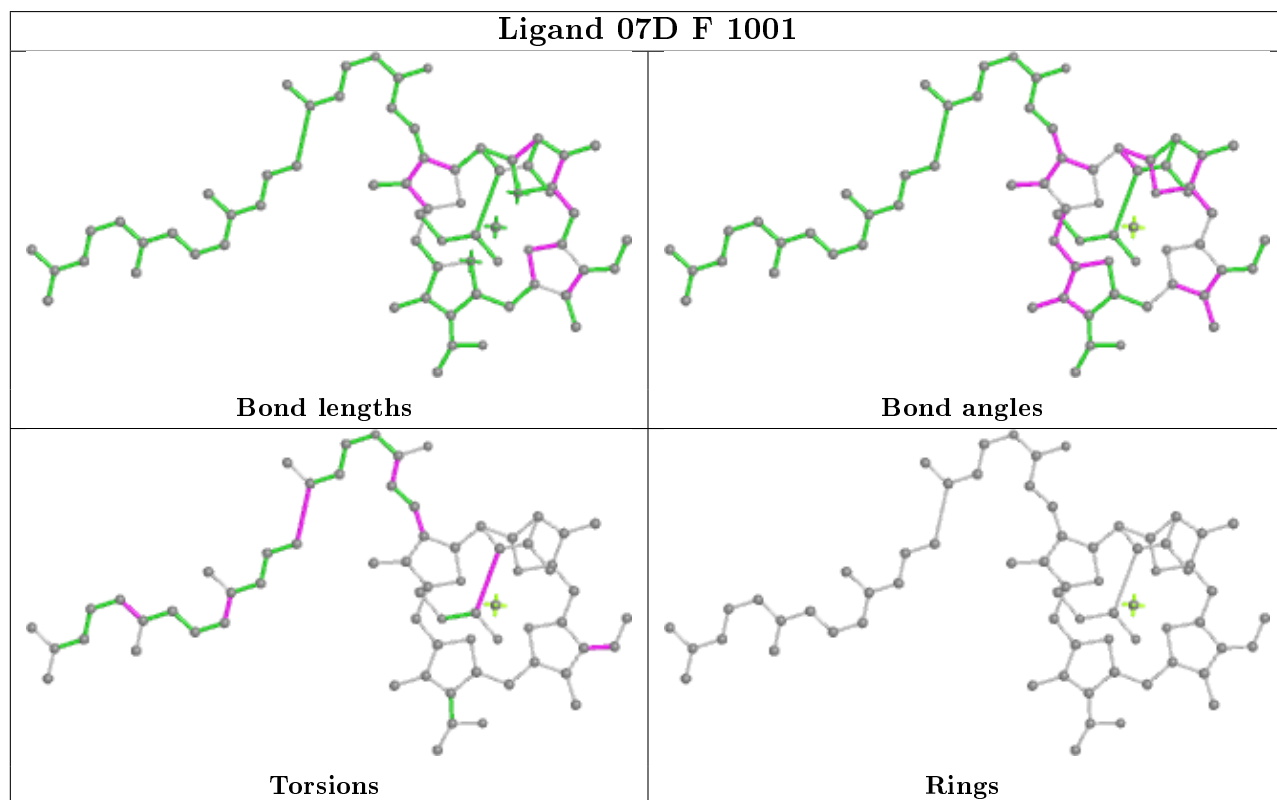
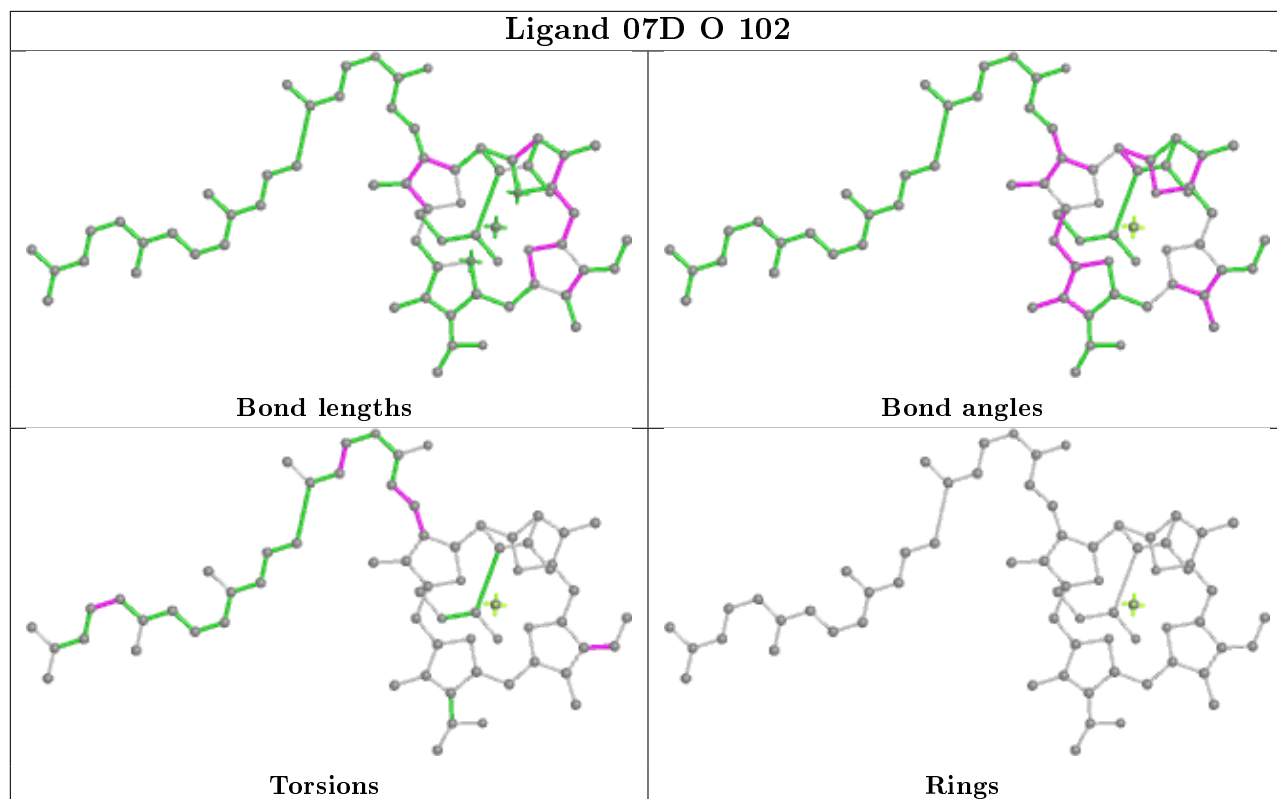


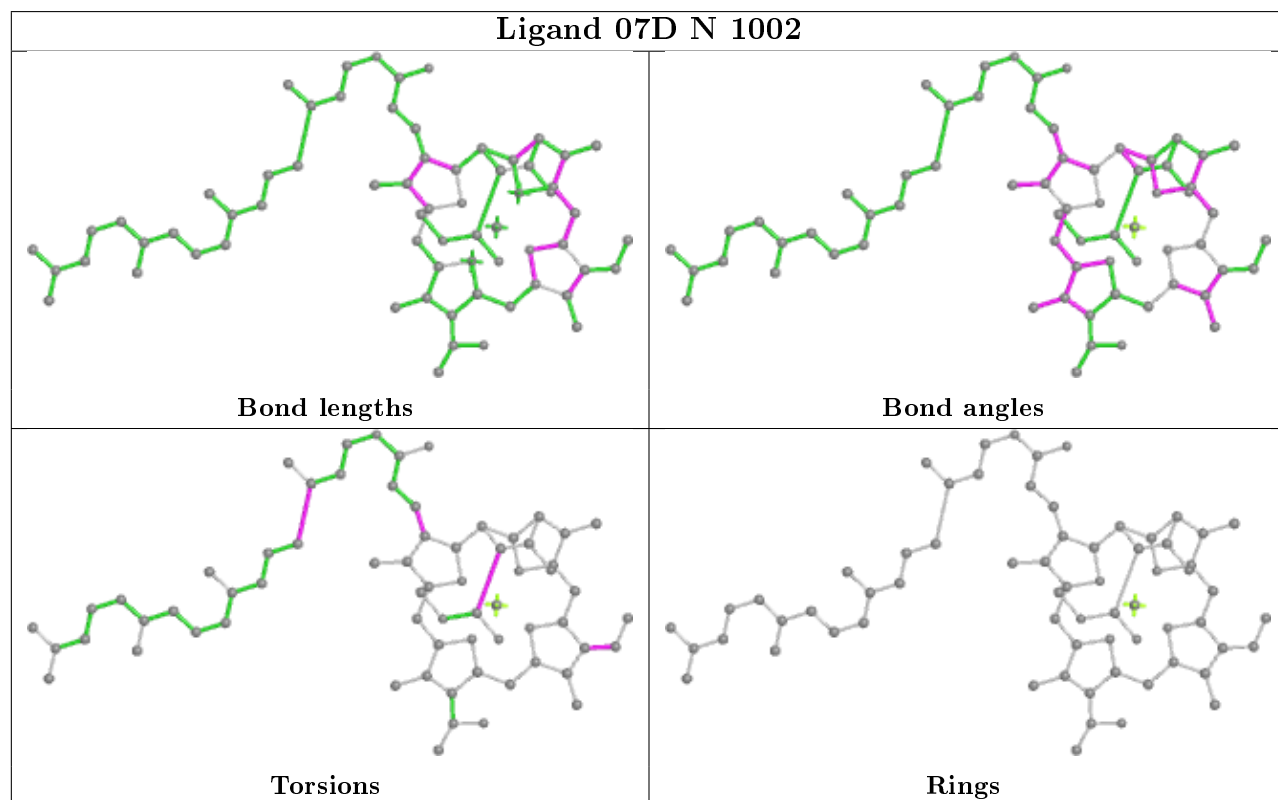
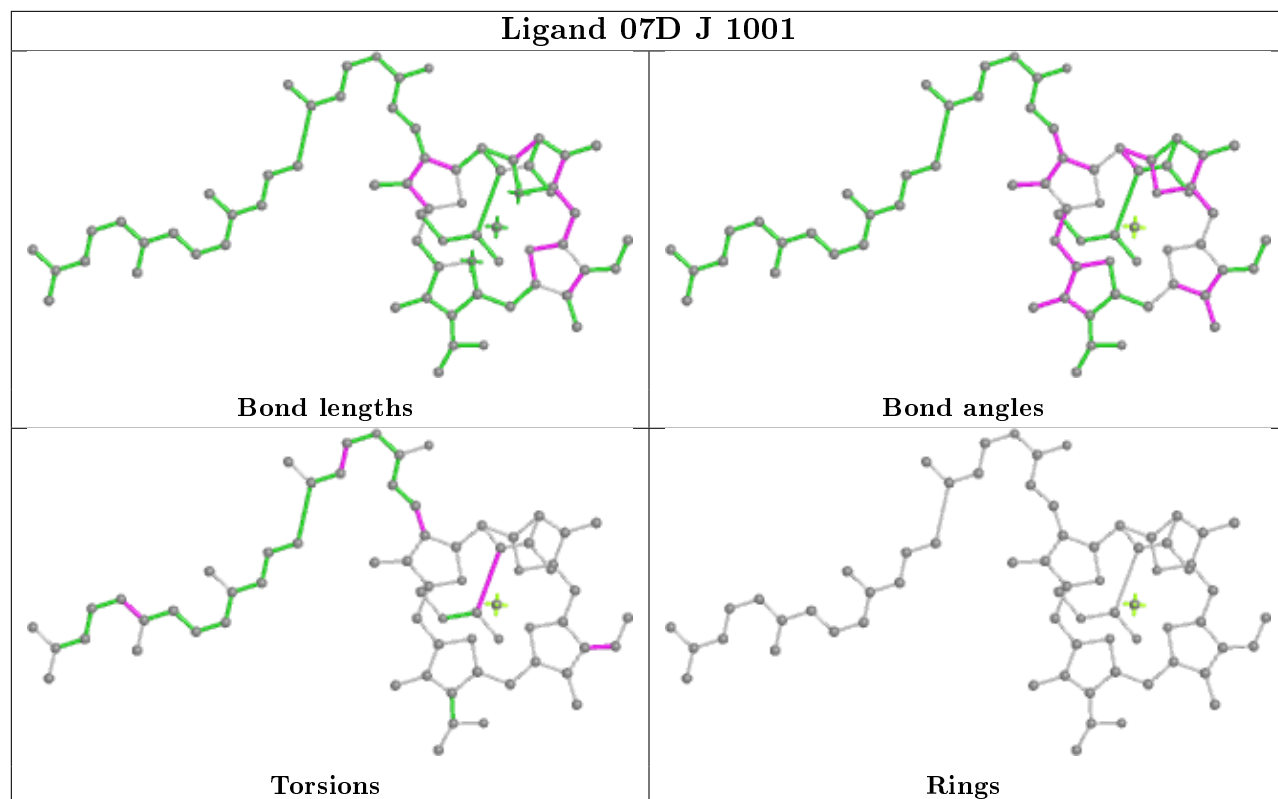


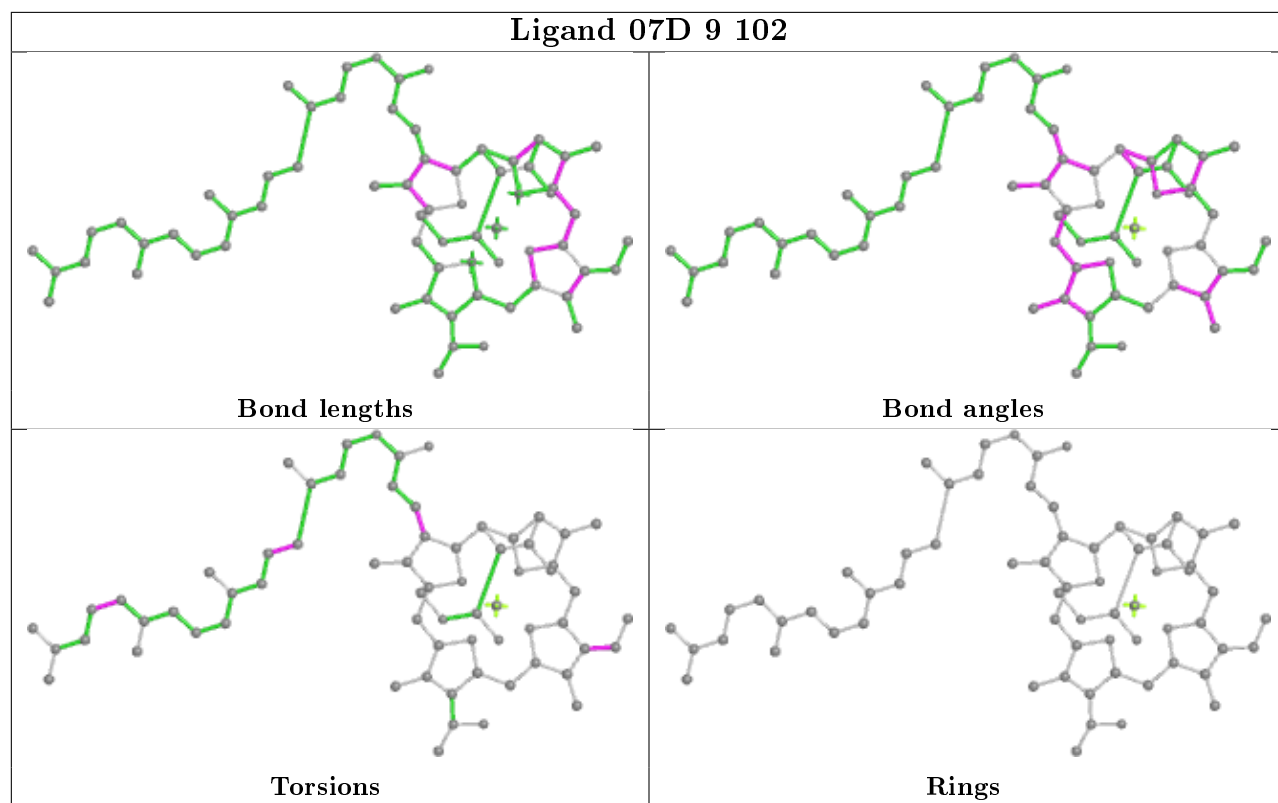
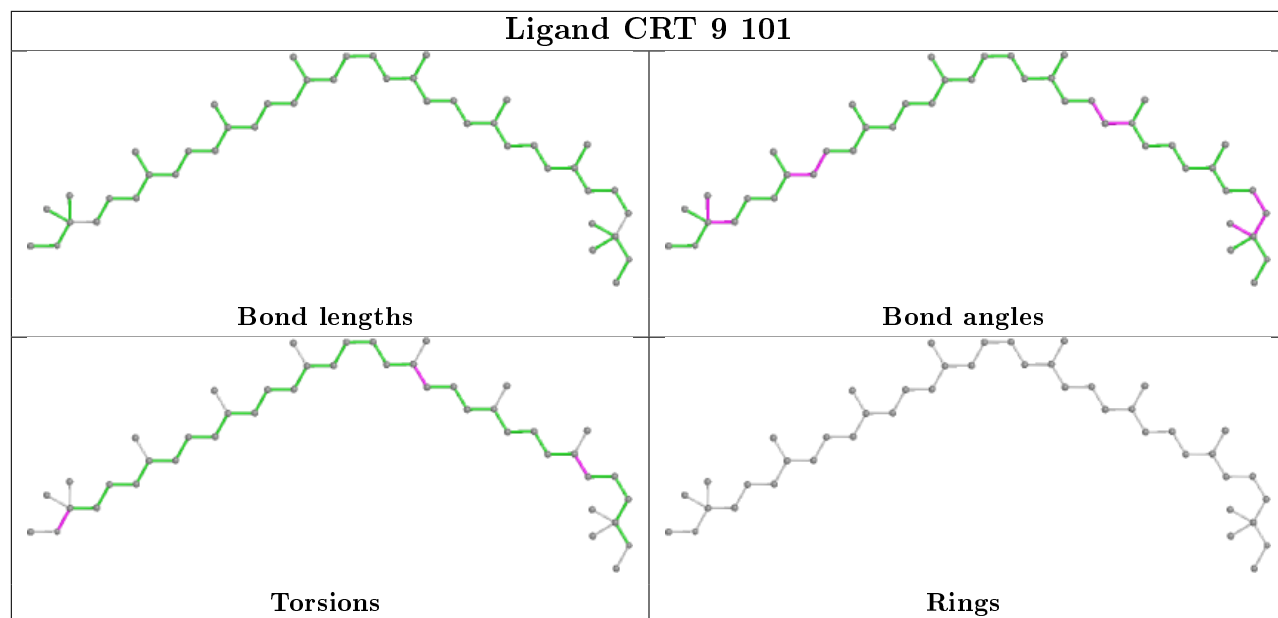


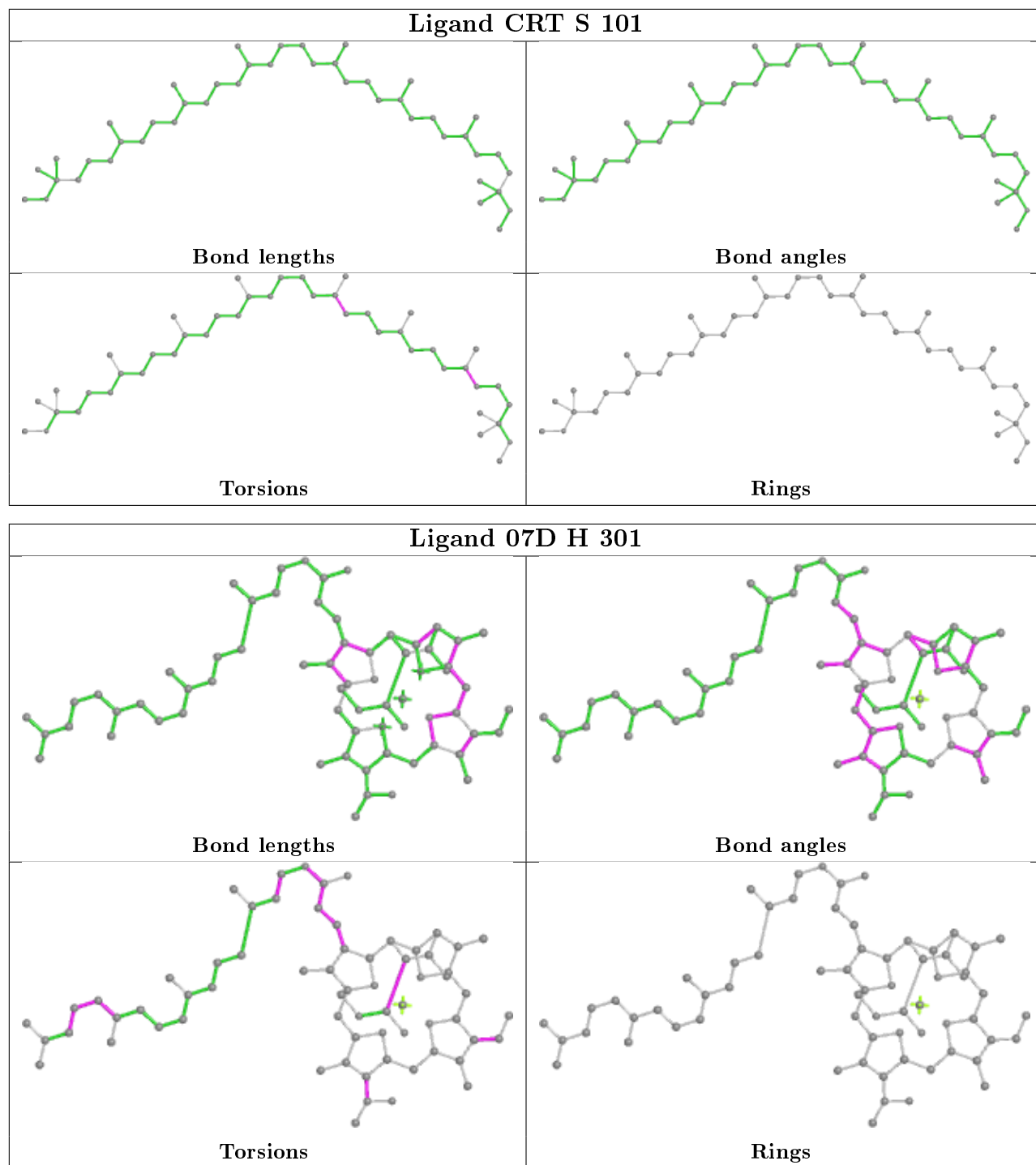


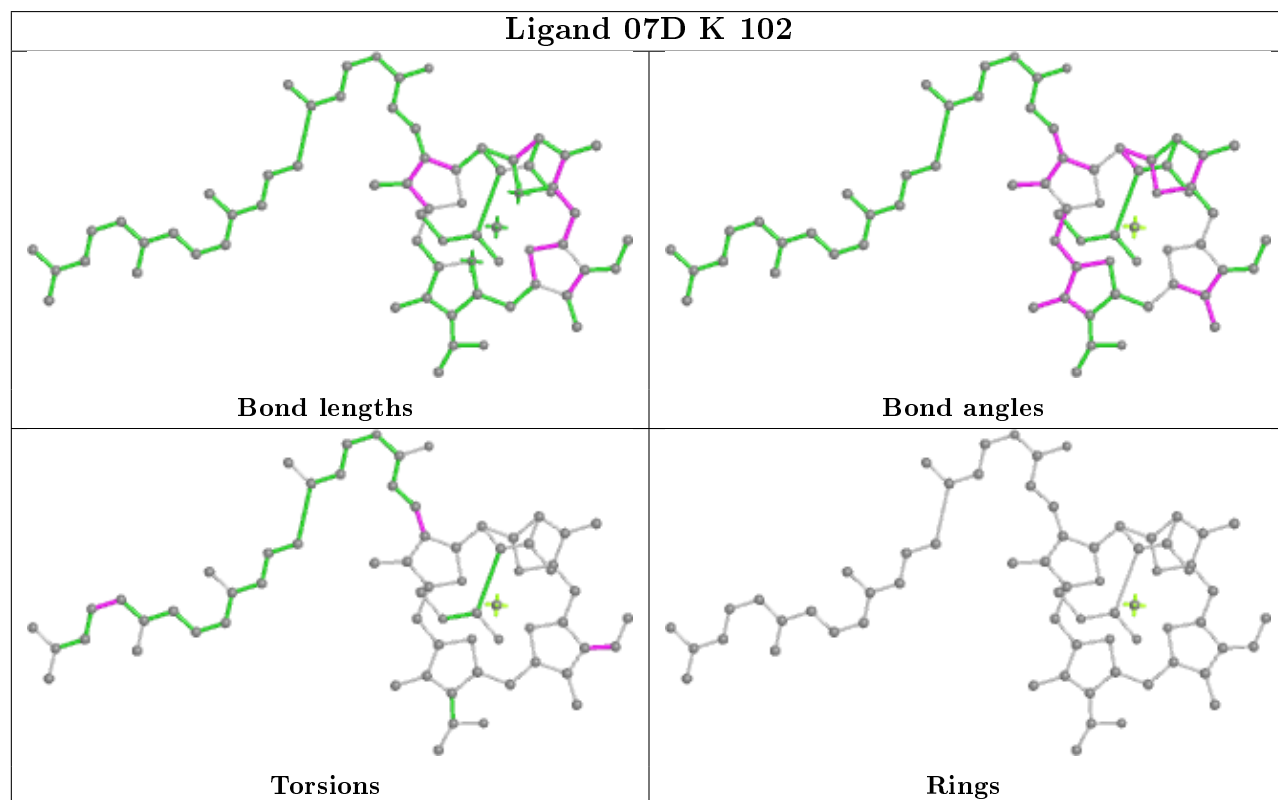
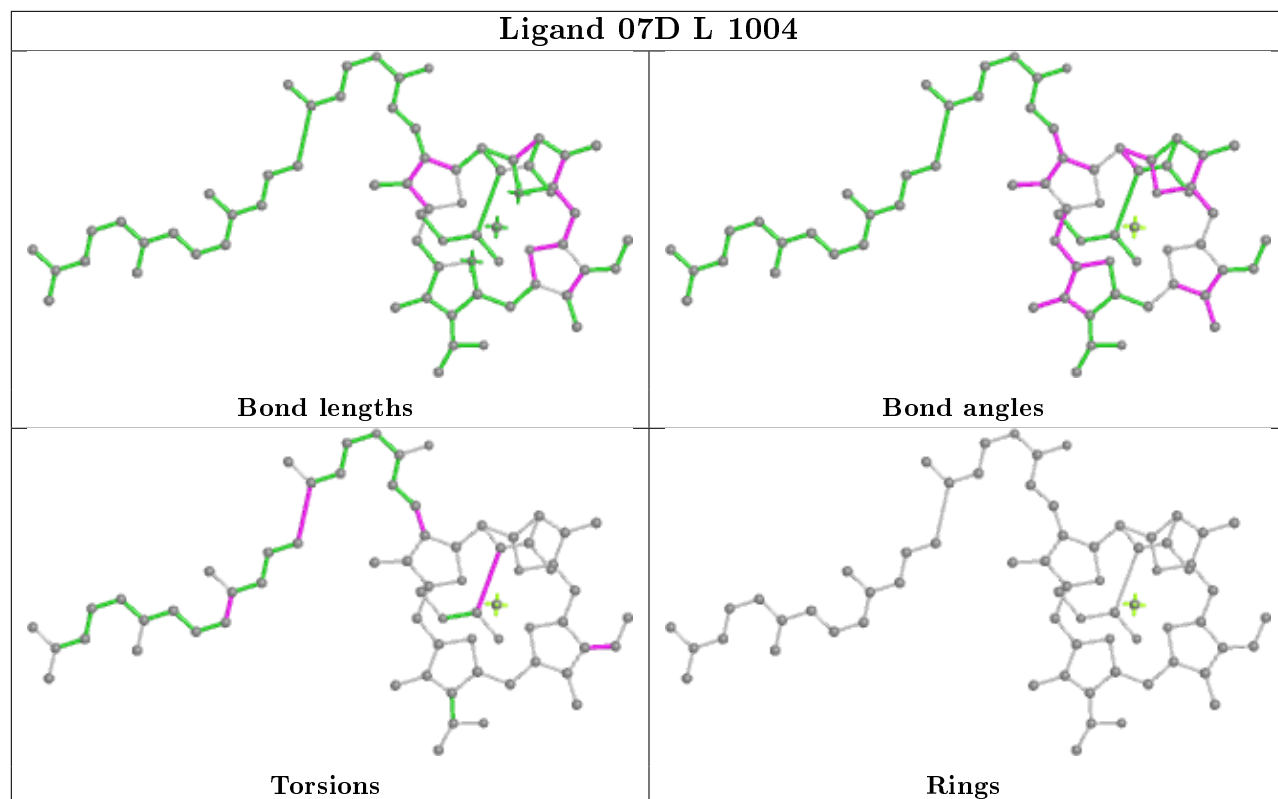


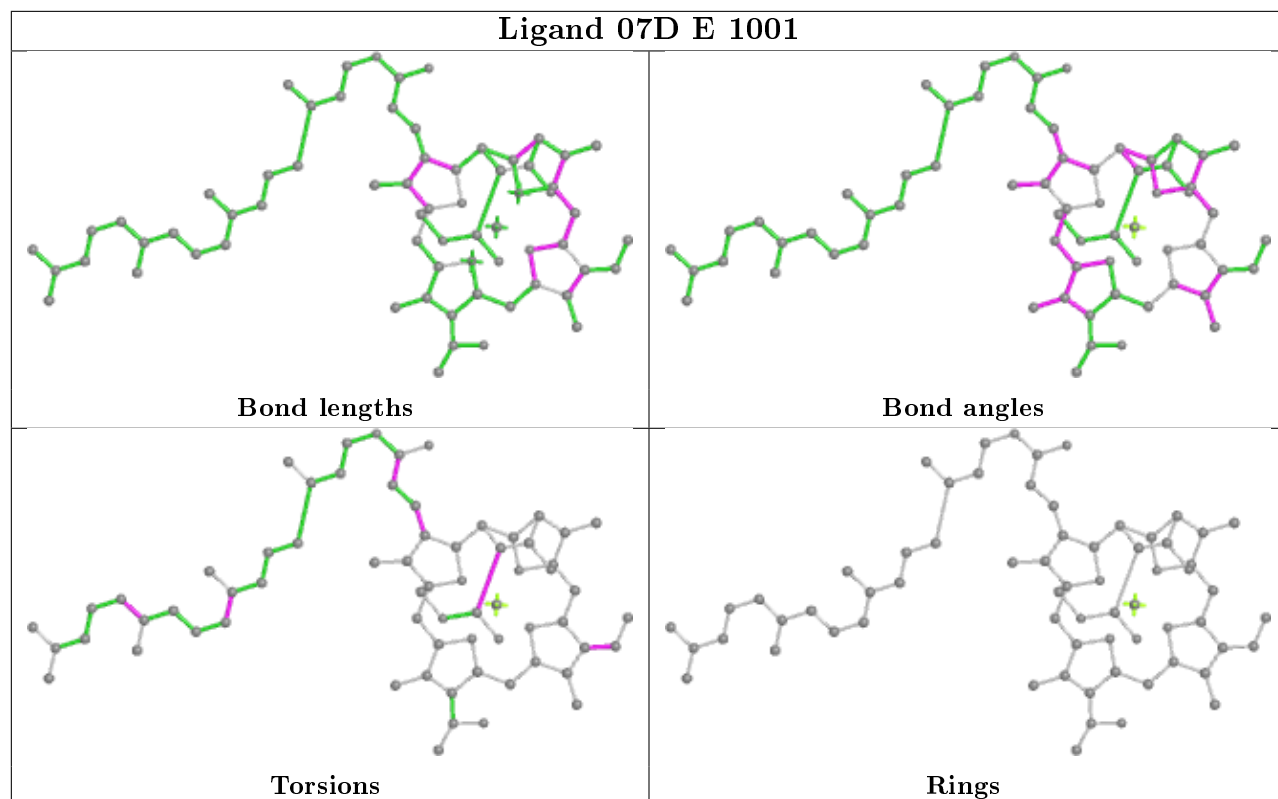


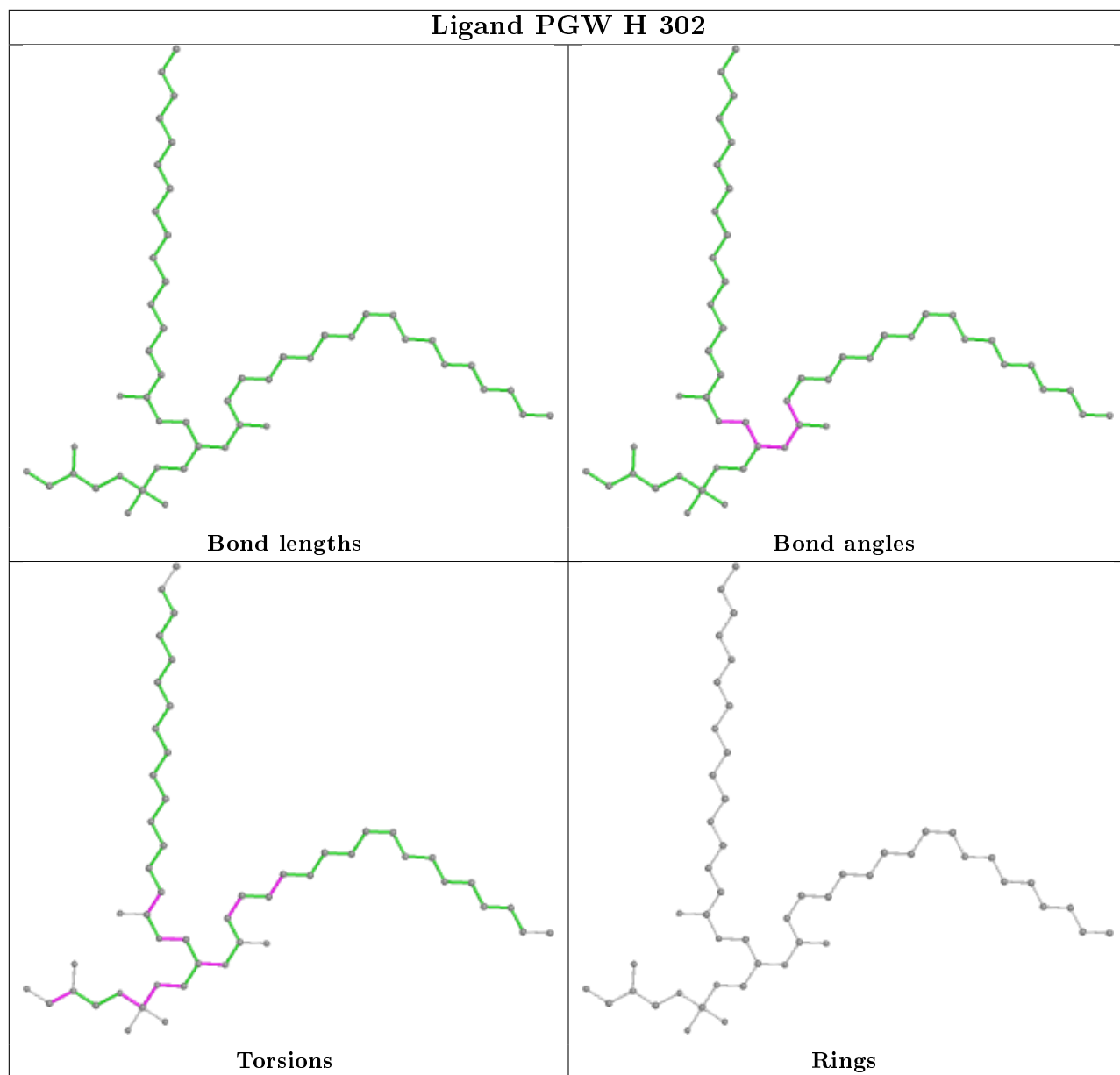


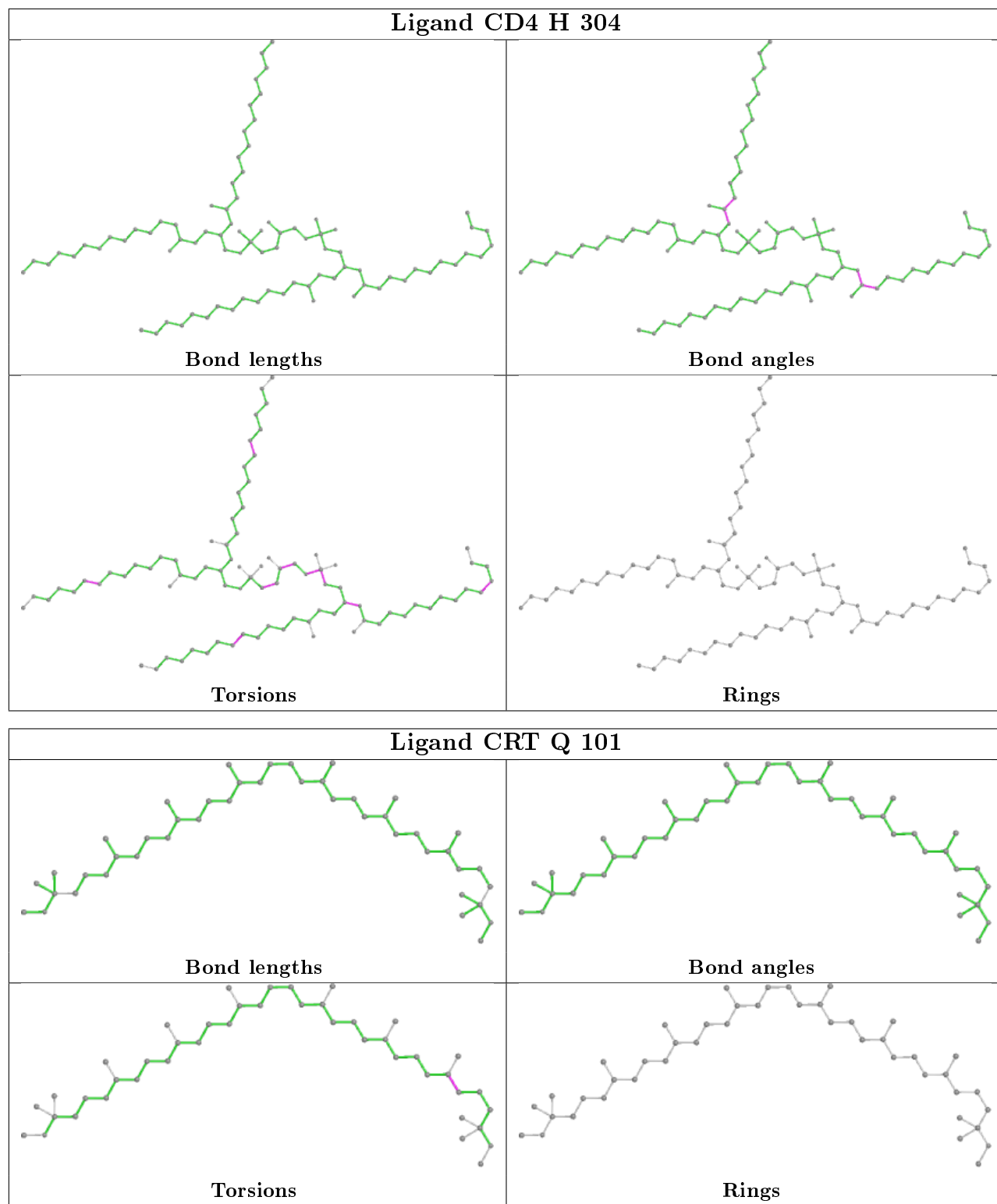




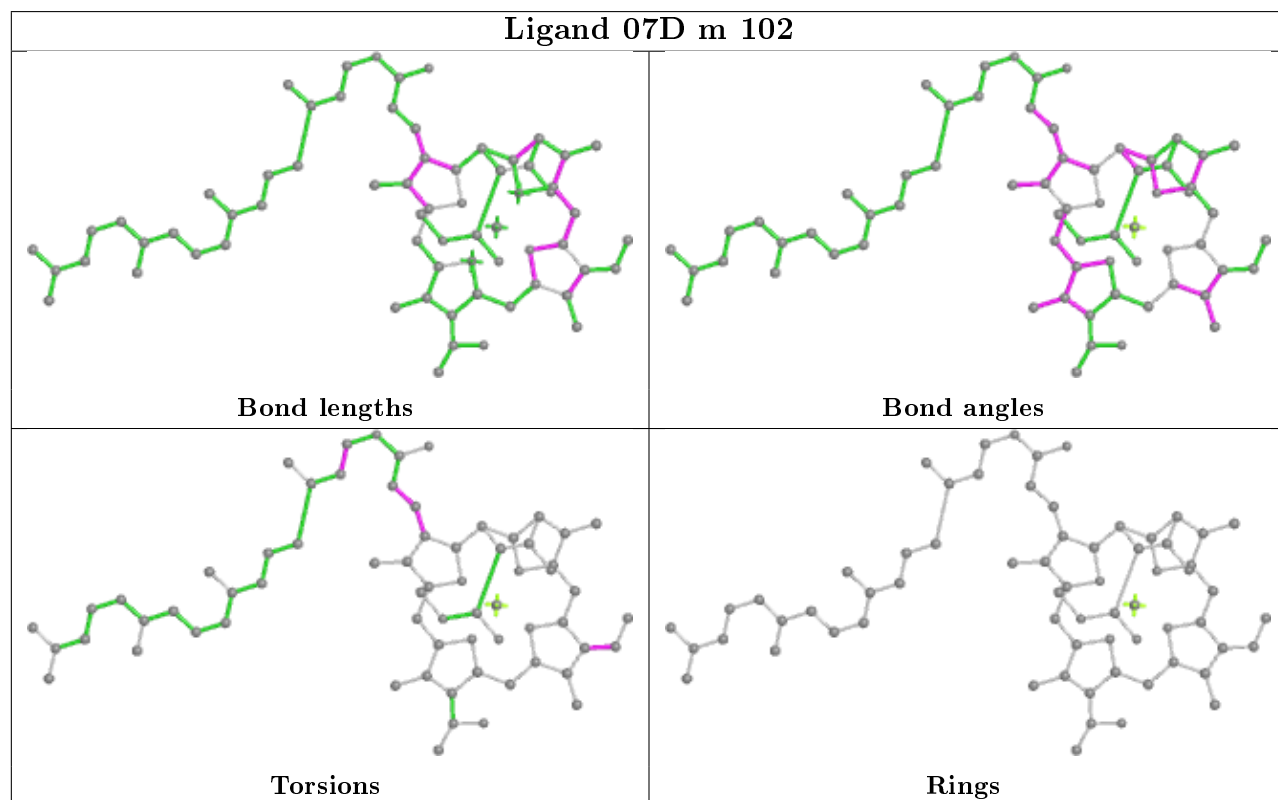
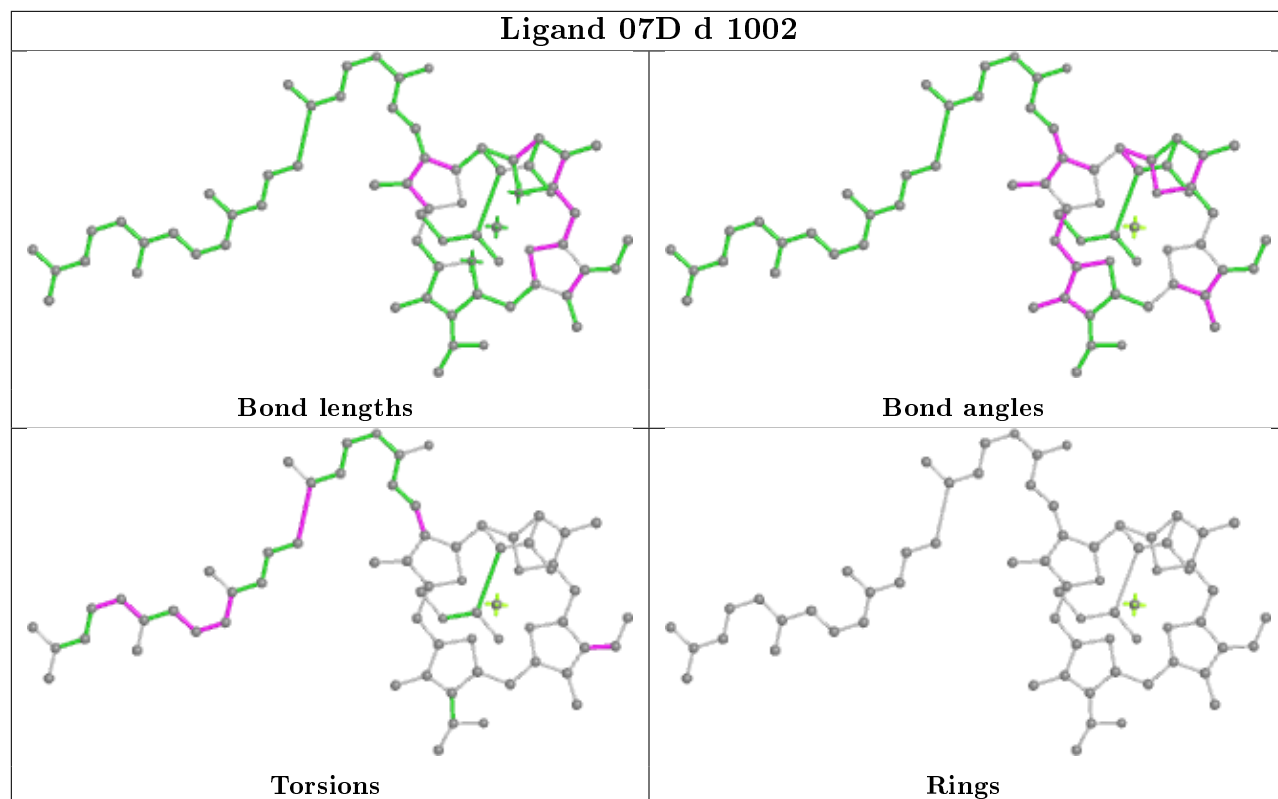


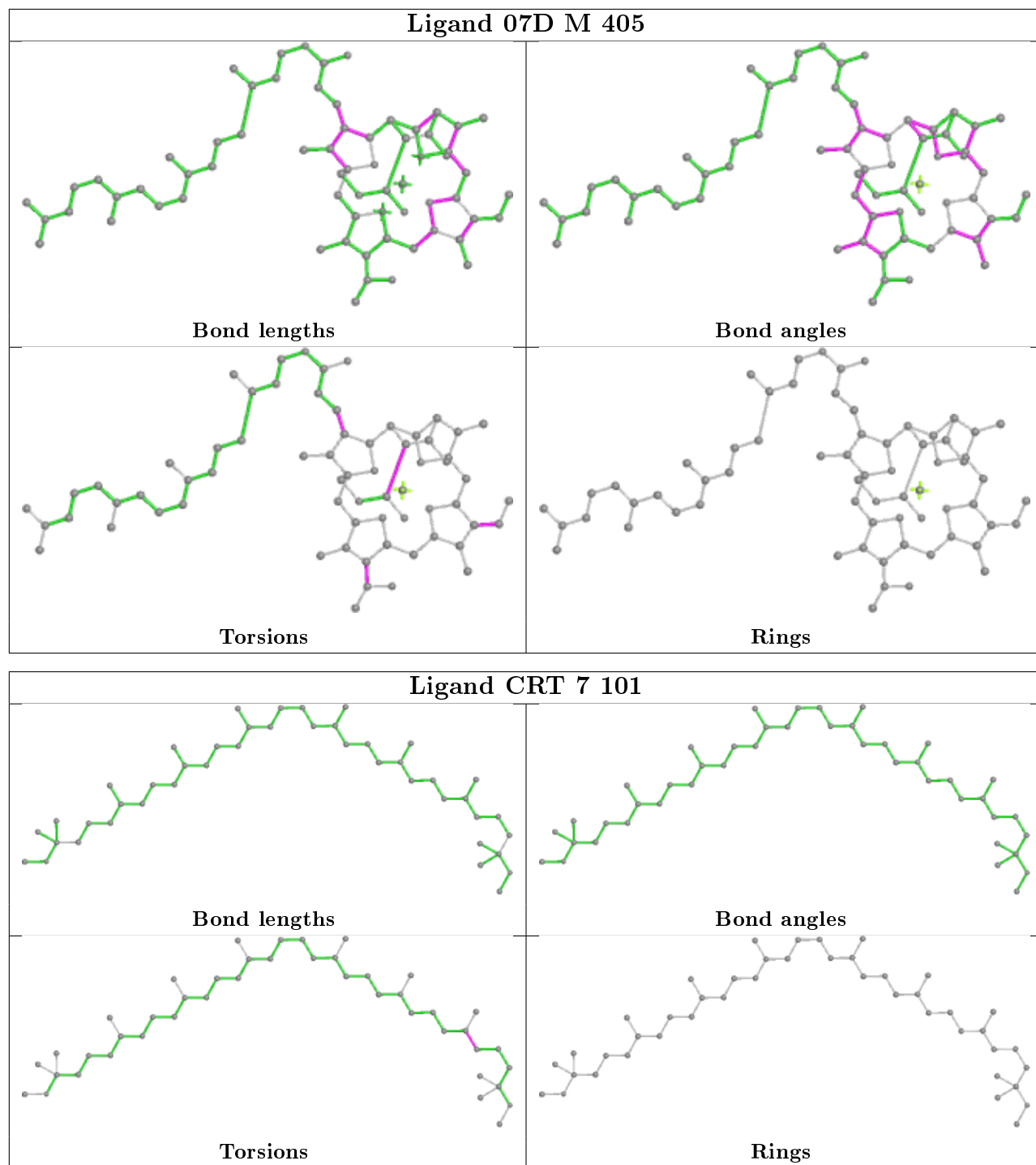


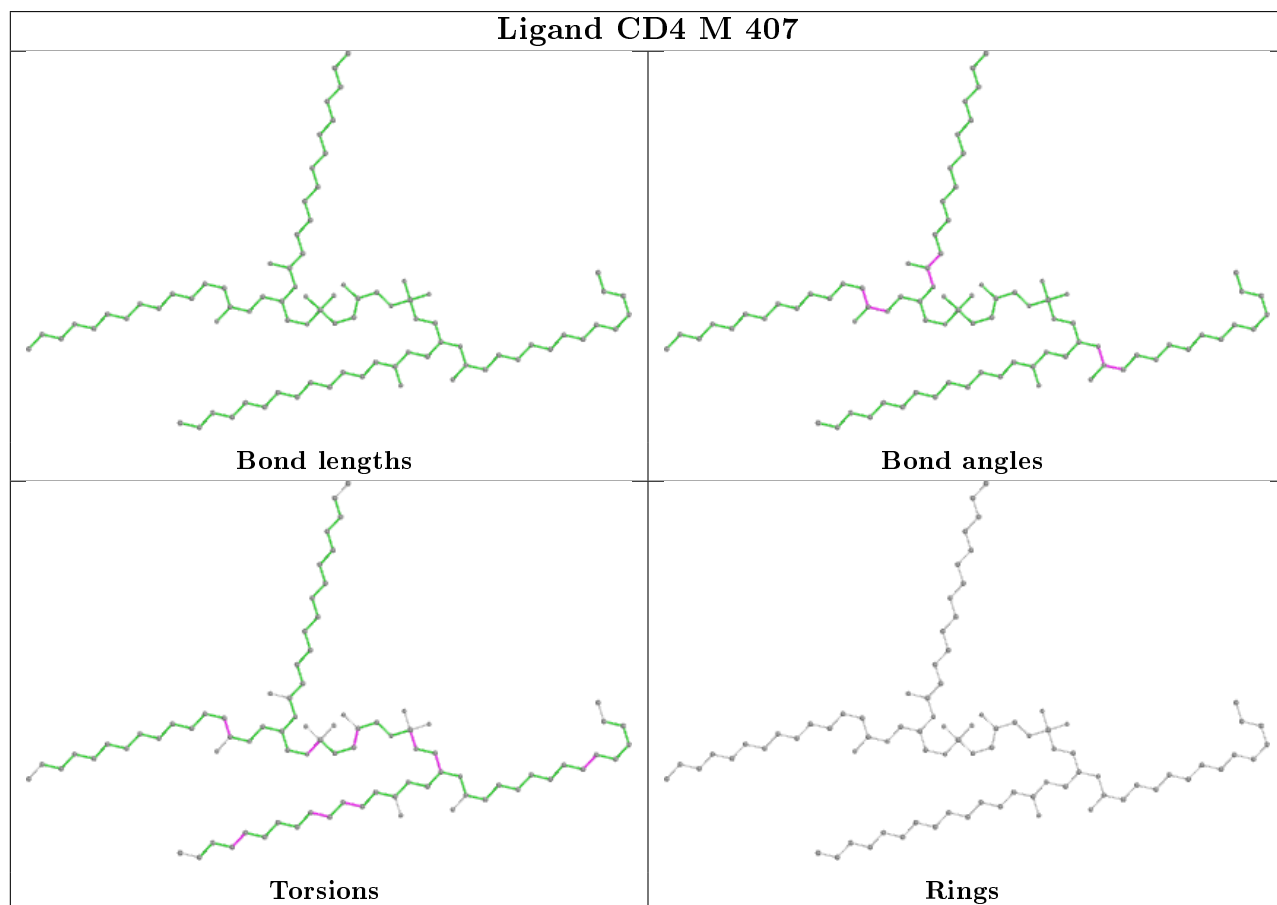
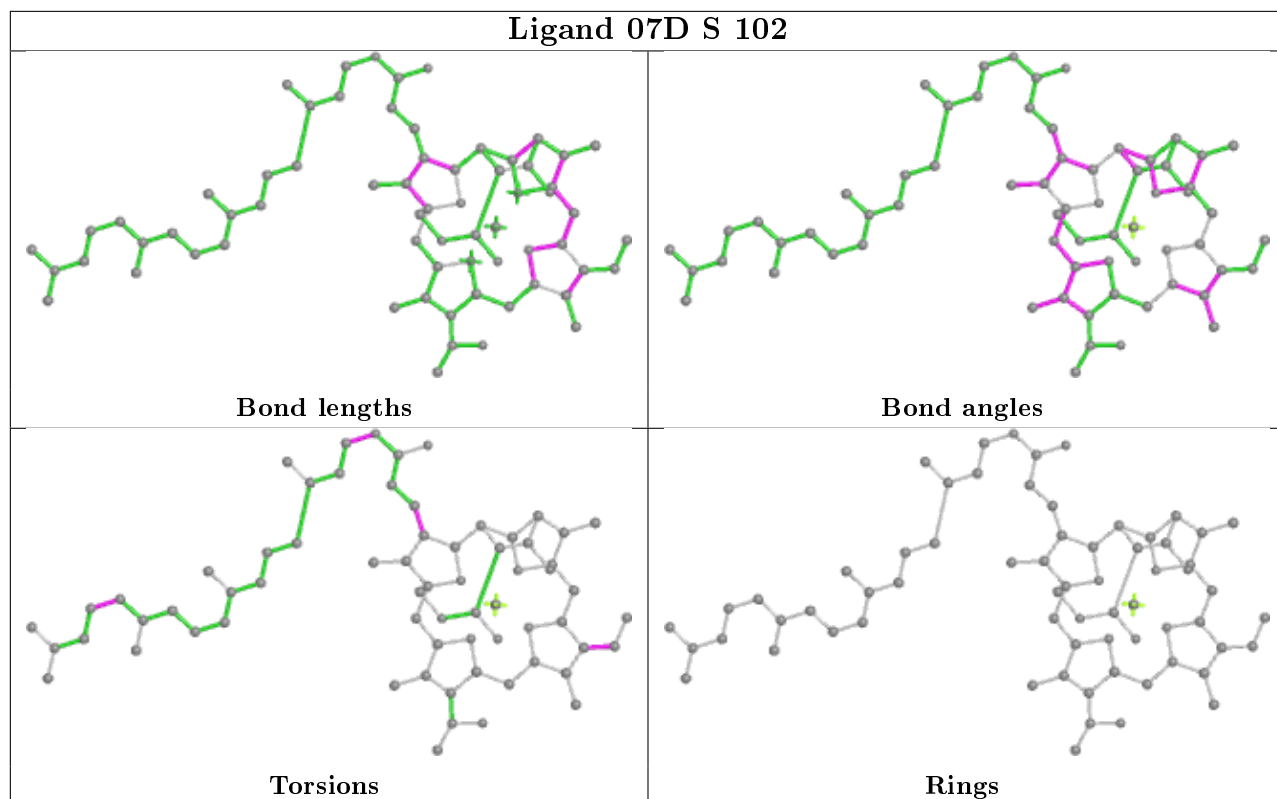


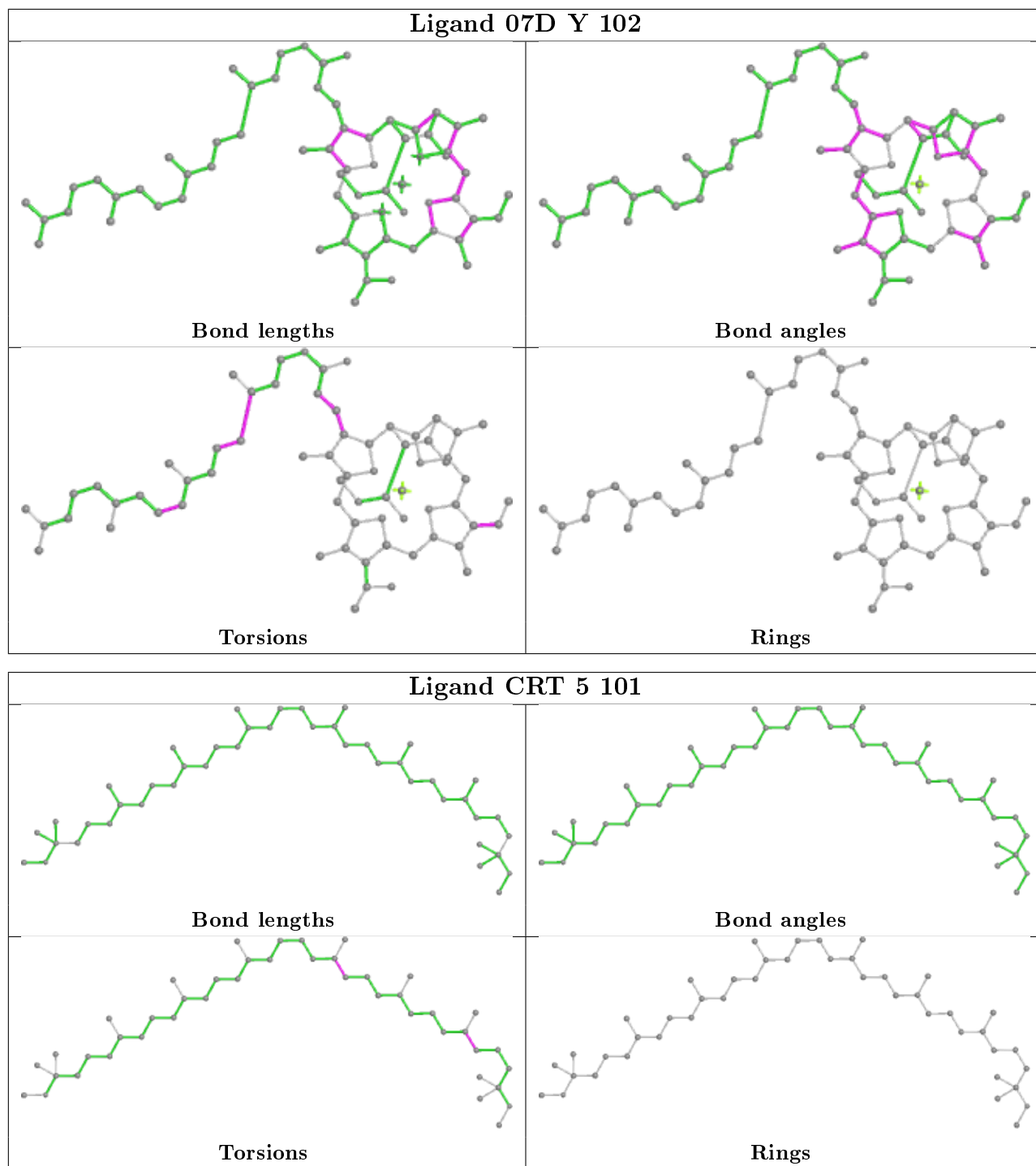


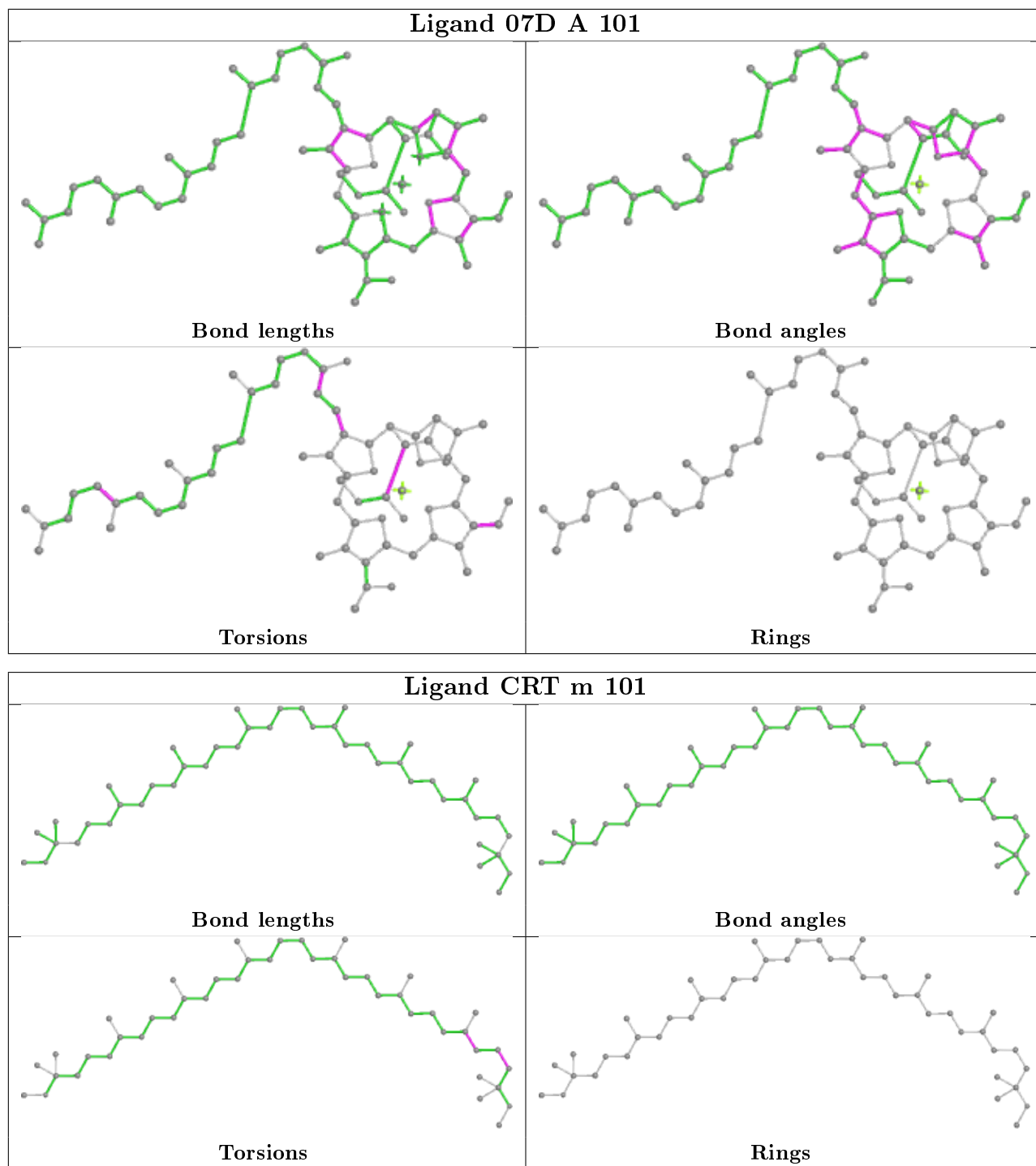


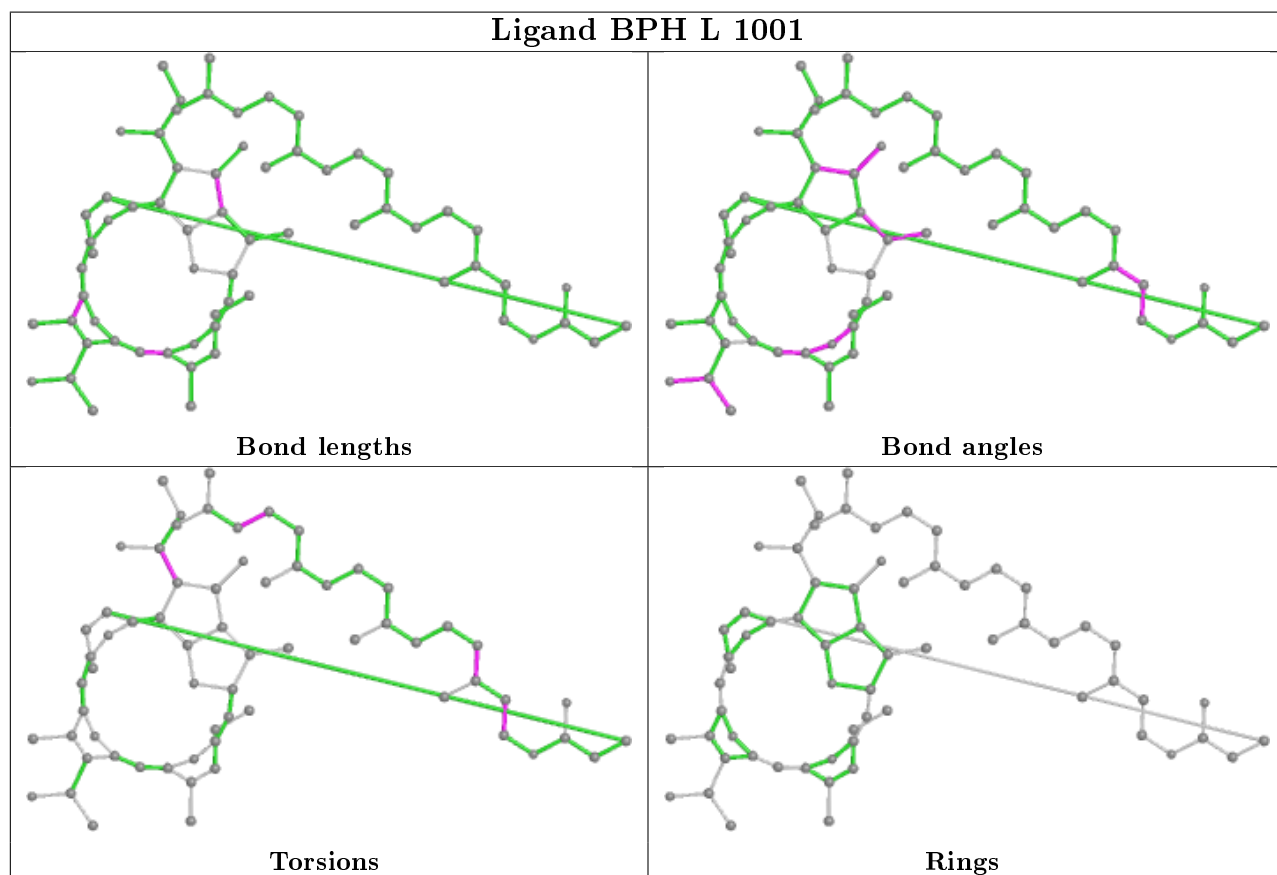
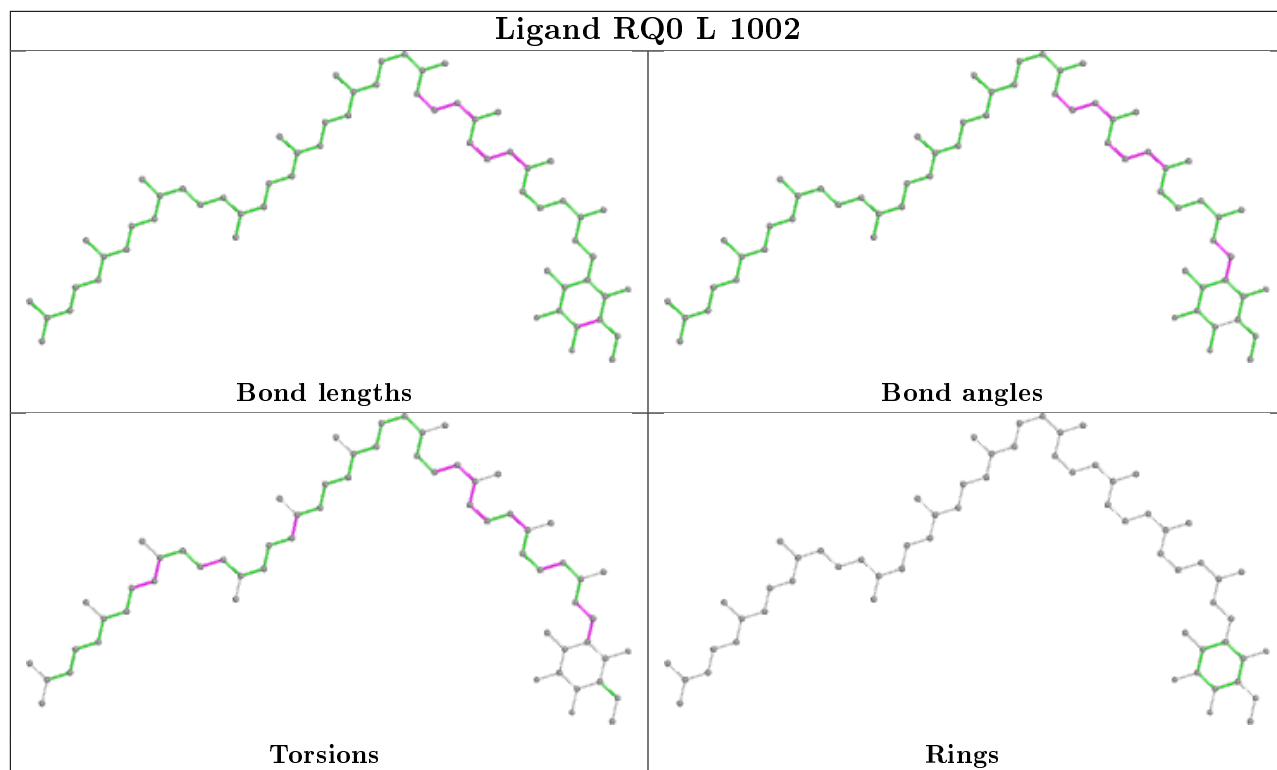


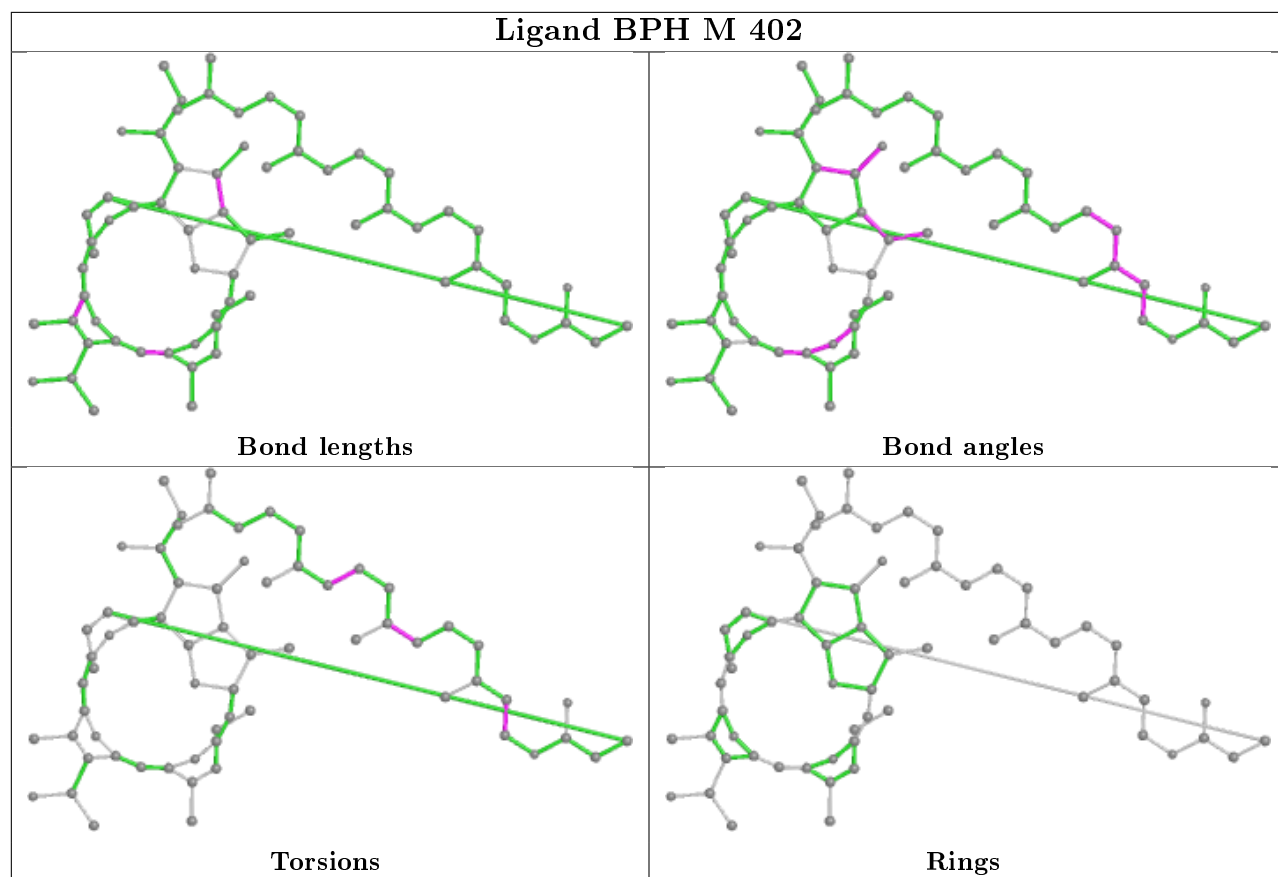
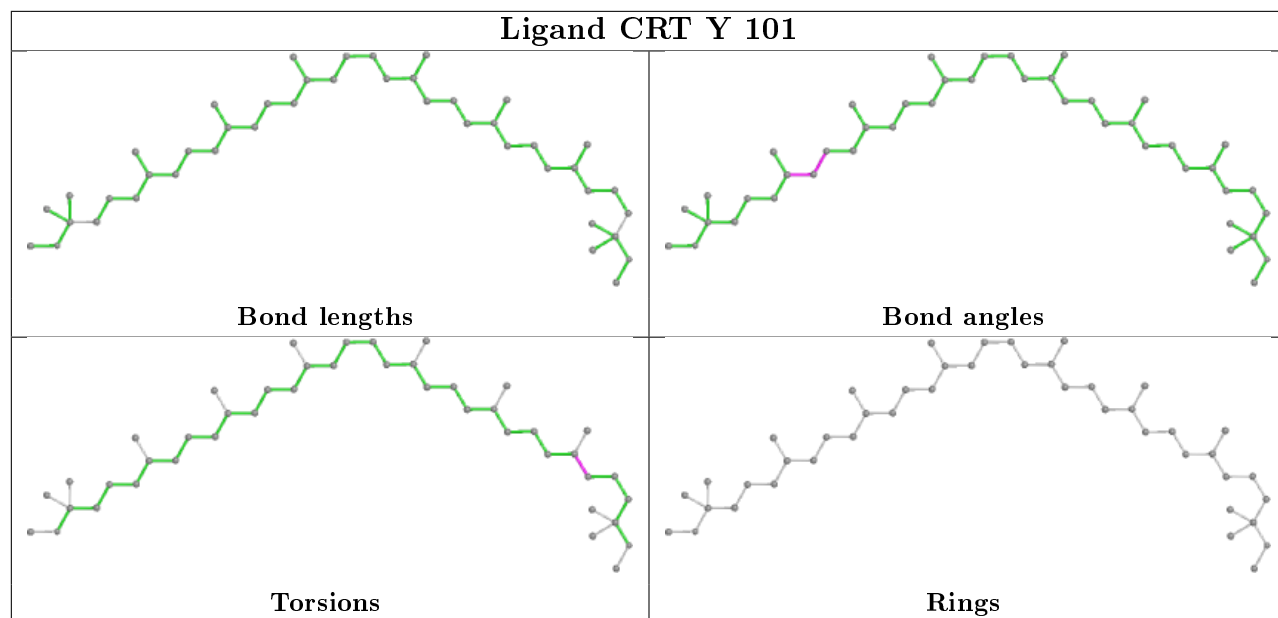


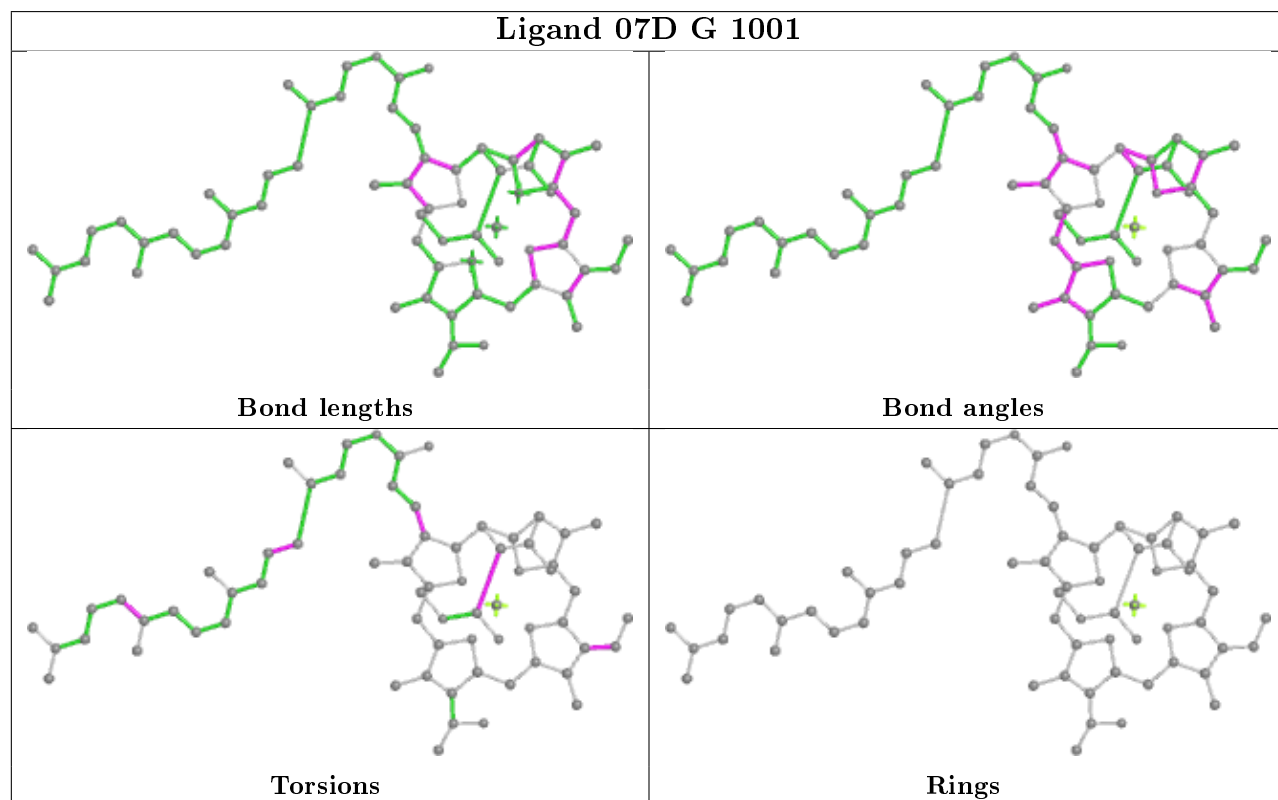
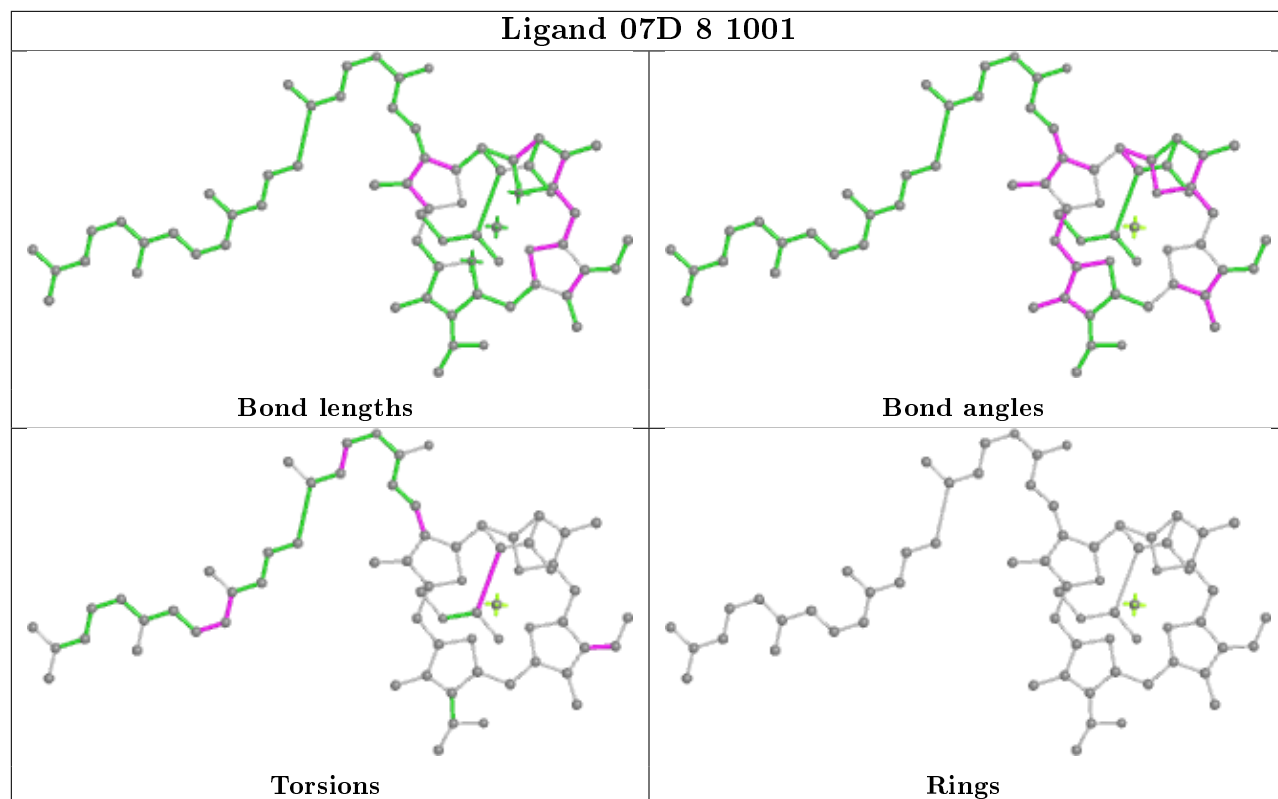




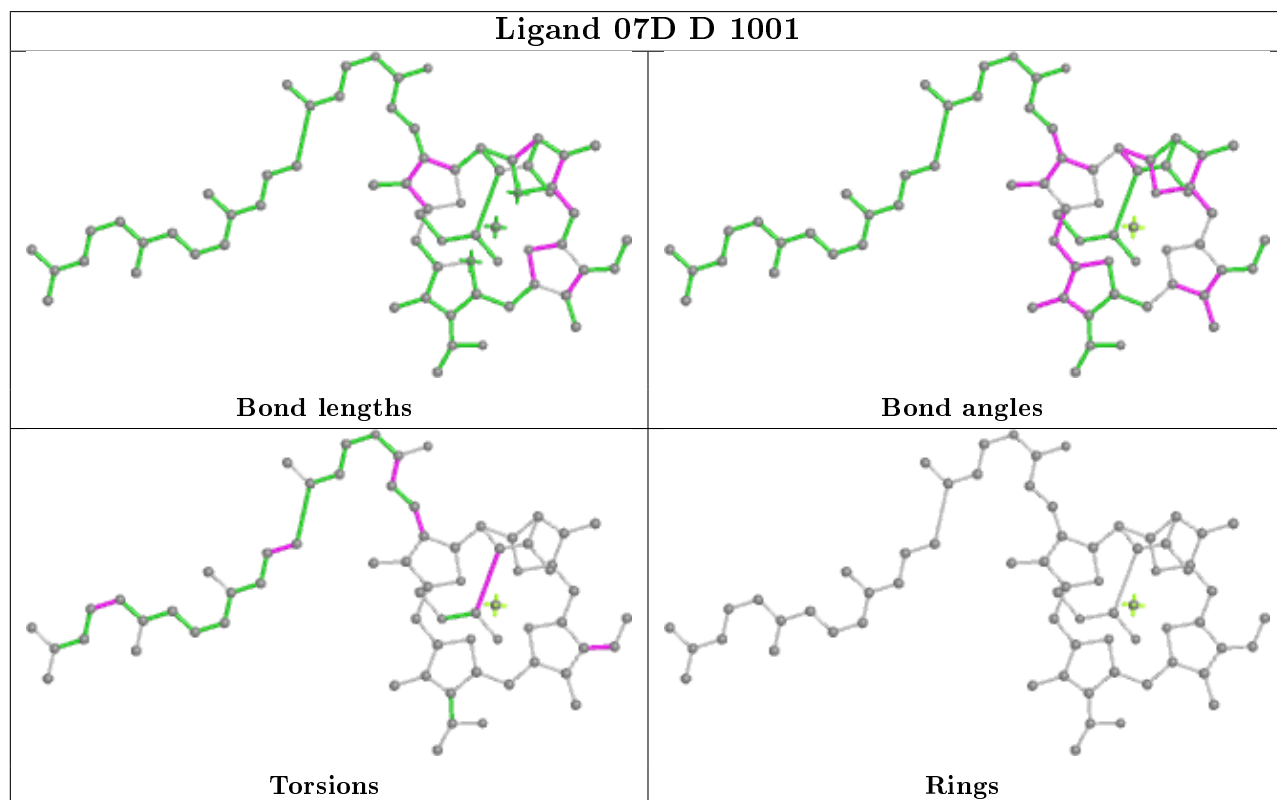
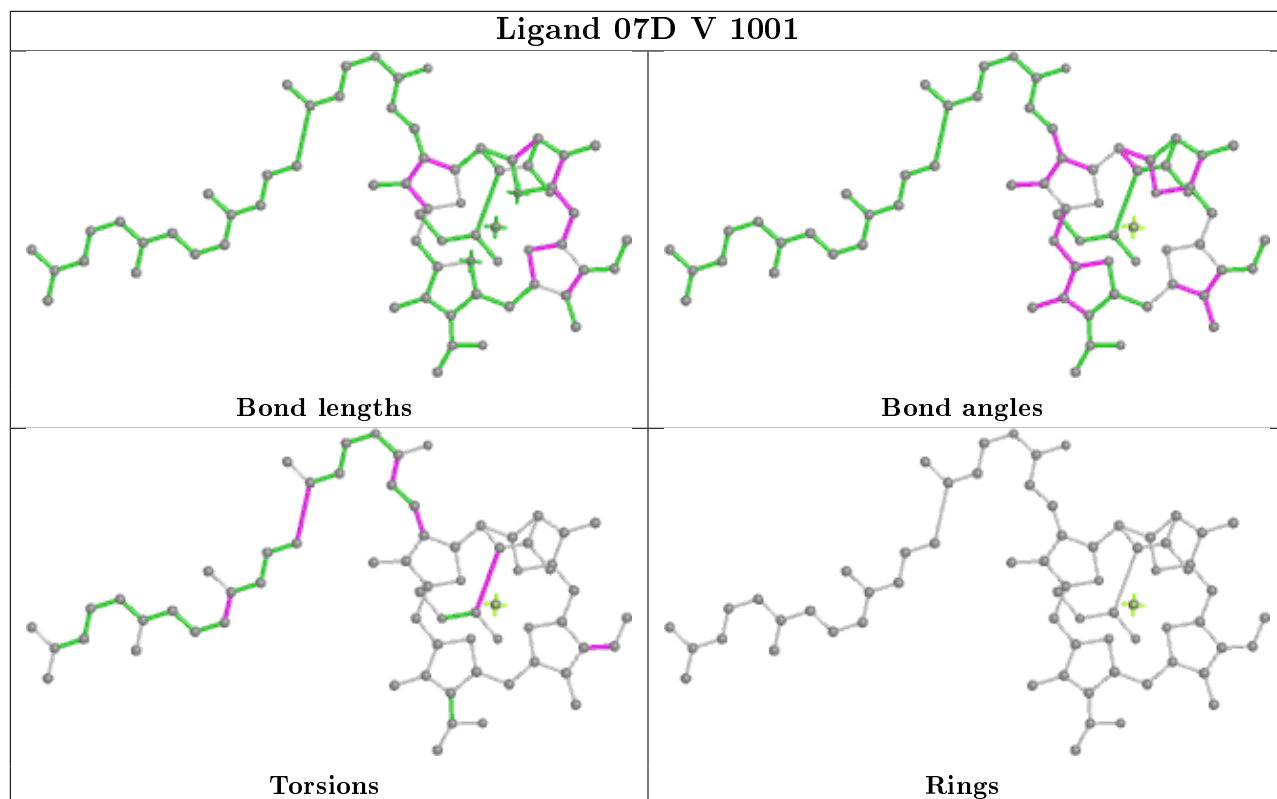


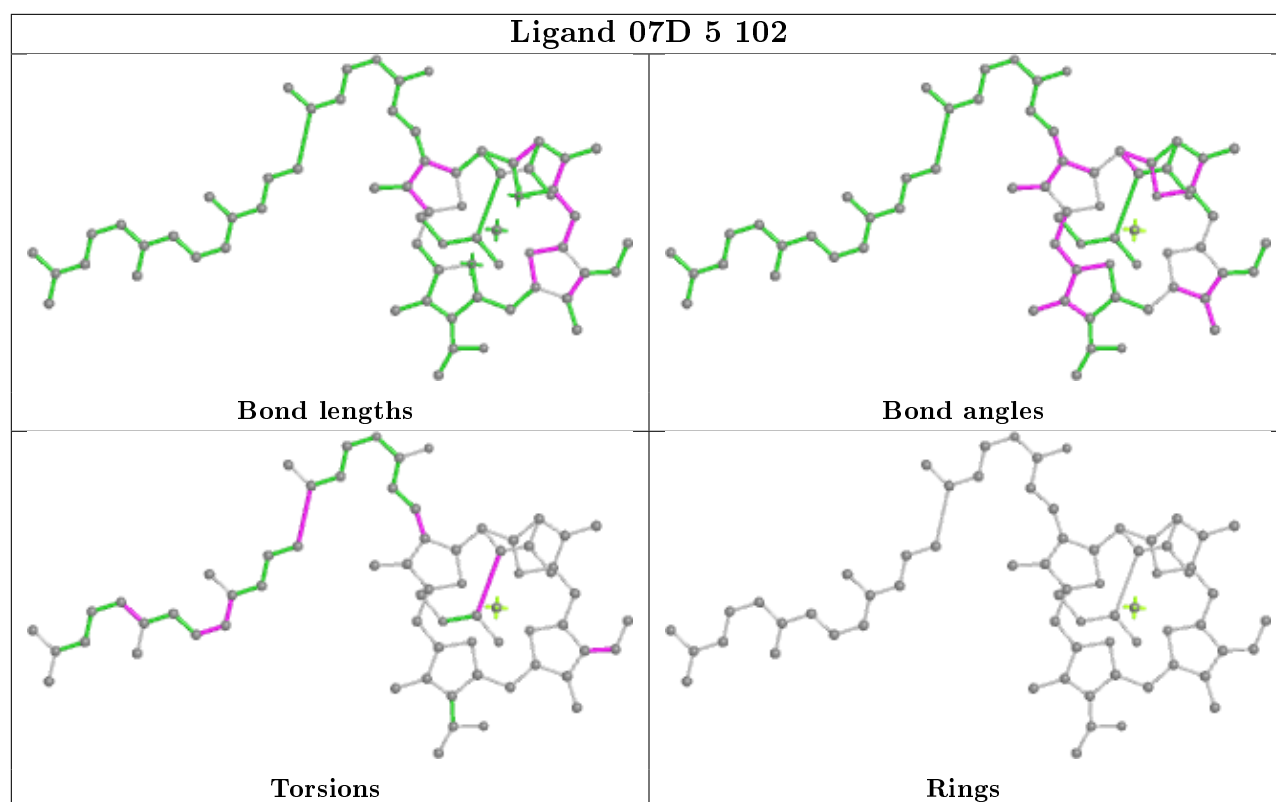












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

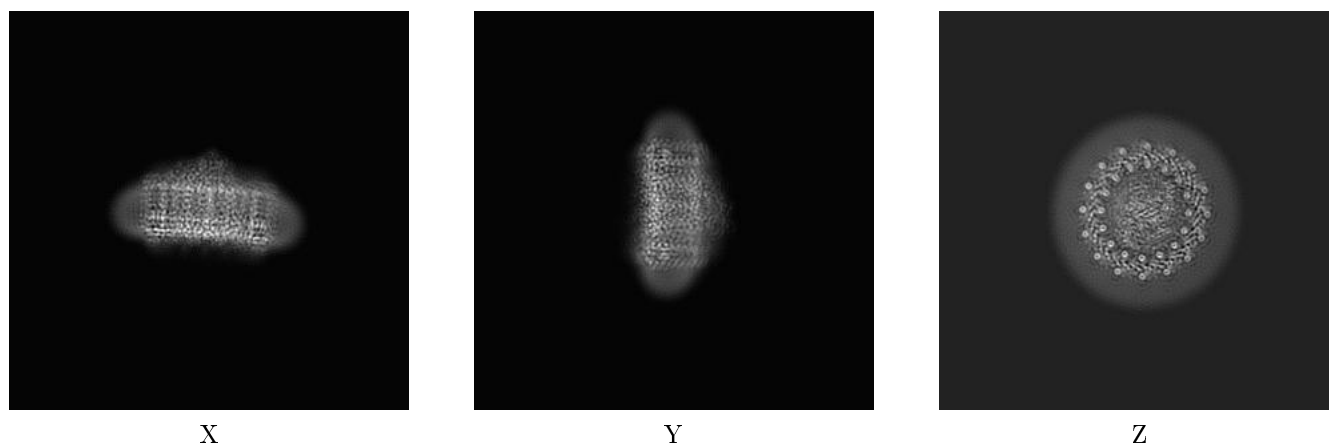
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13110. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

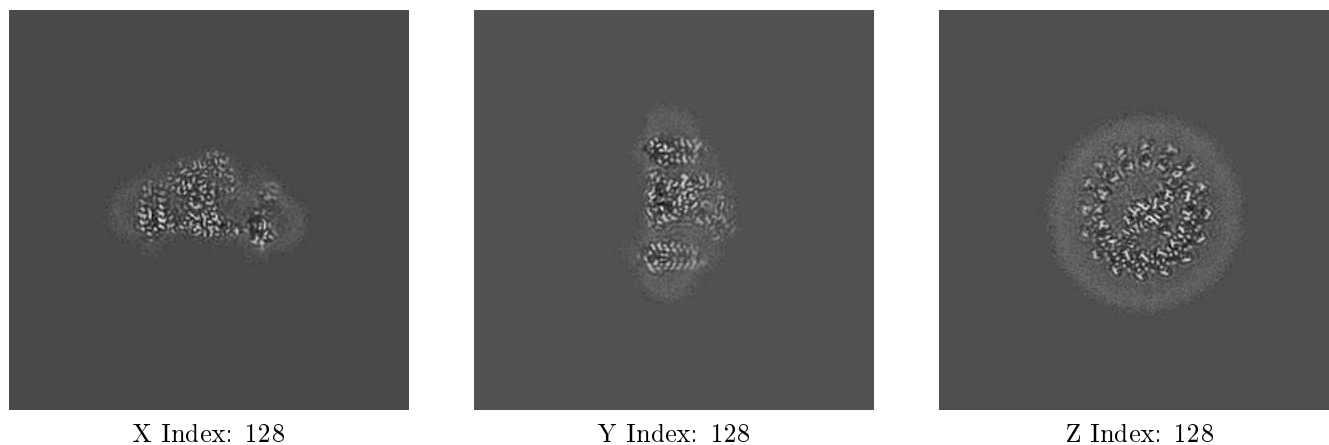
#### 6.1.1 Primary map



The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

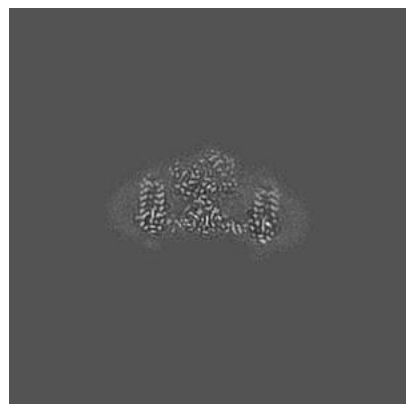
#### 6.2.1 Primary map



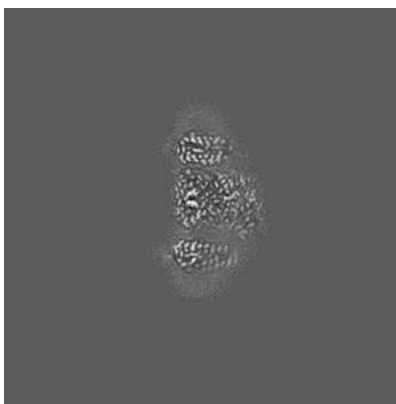
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

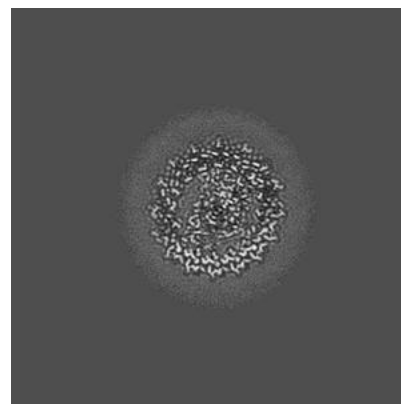
### 6.3.1 Primary map



X Index: 131



Y Index: 126



Z Index: 115

The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

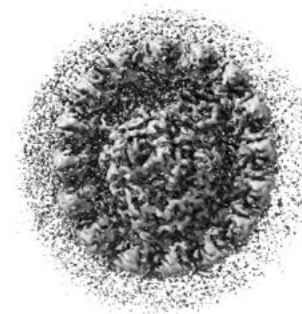
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0165. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

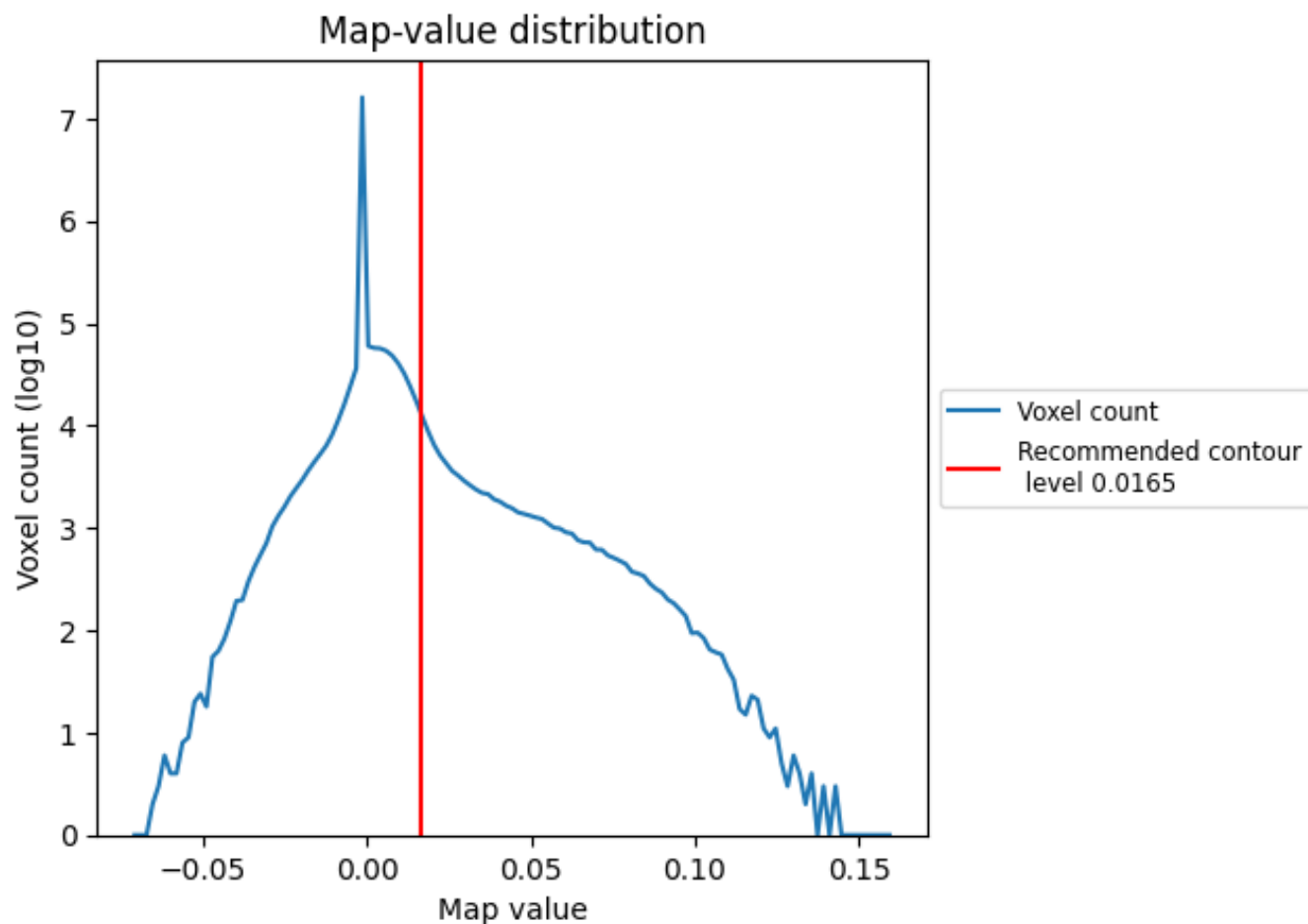
## 6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

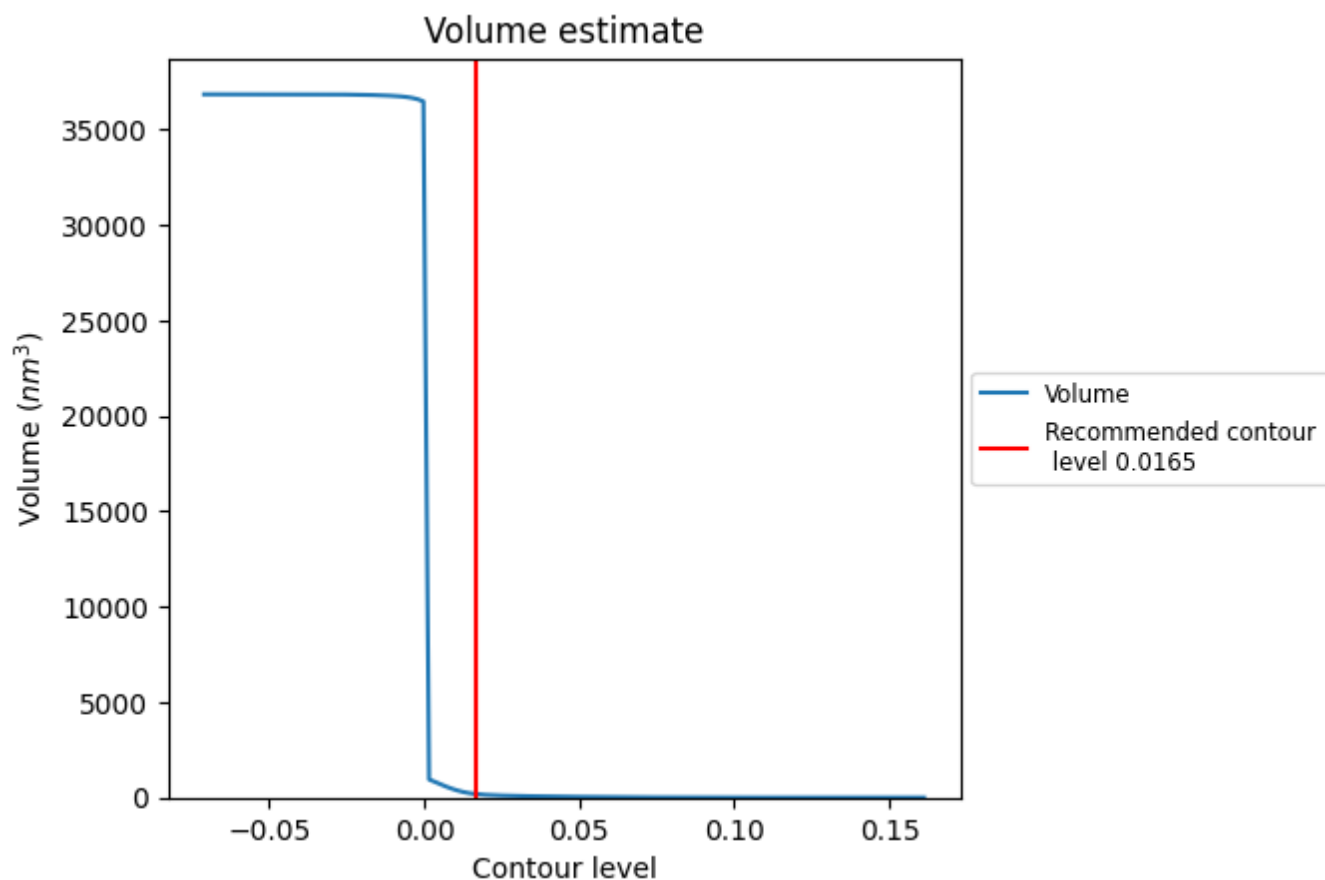
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

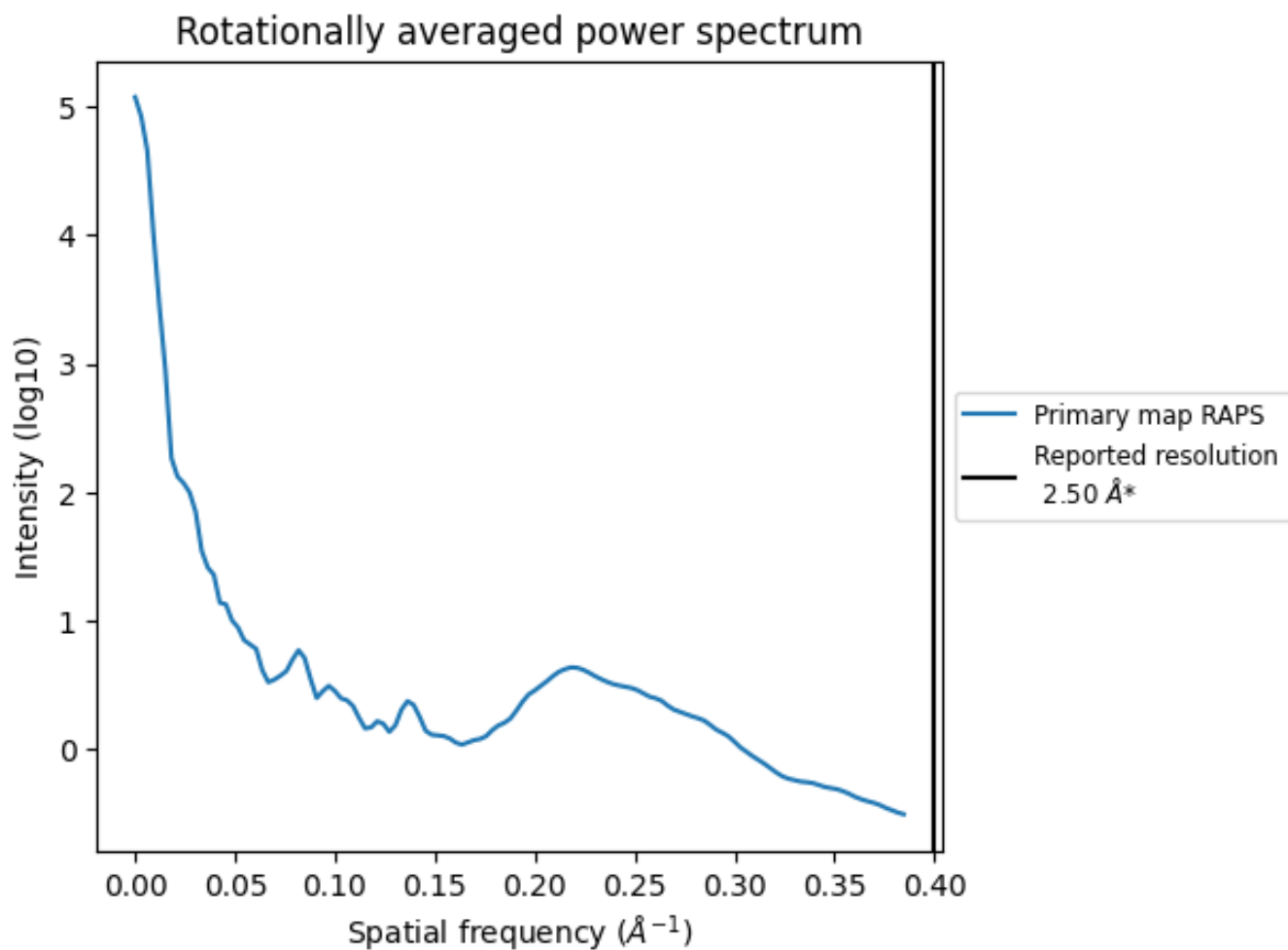
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 189 nm<sup>3</sup>; this corresponds to an approximate mass of 171 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum [\(i\)](#)



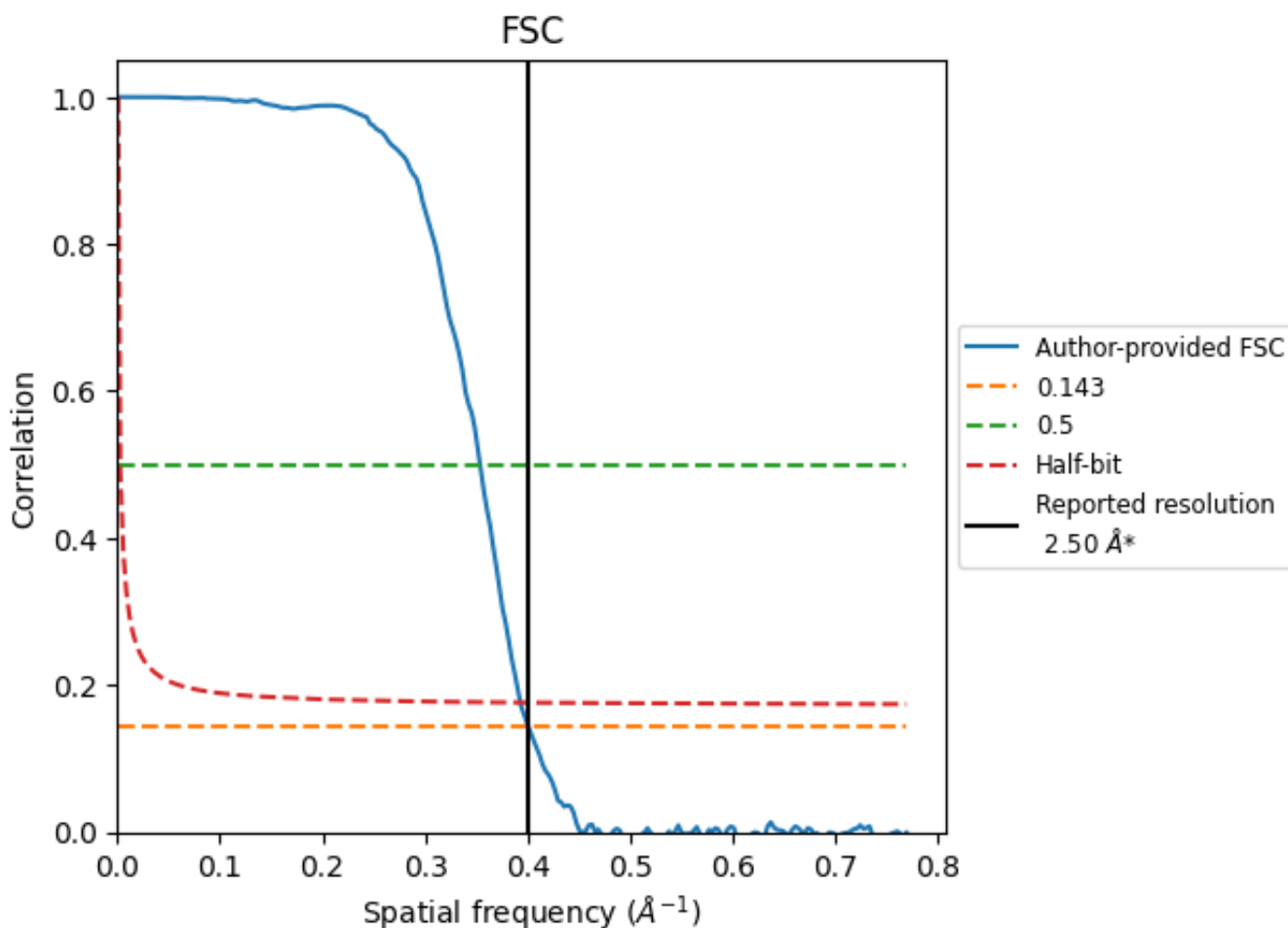
\*Reported resolution corresponds to spatial frequency of 0.400 Å<sup>-1</sup>



## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.400 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

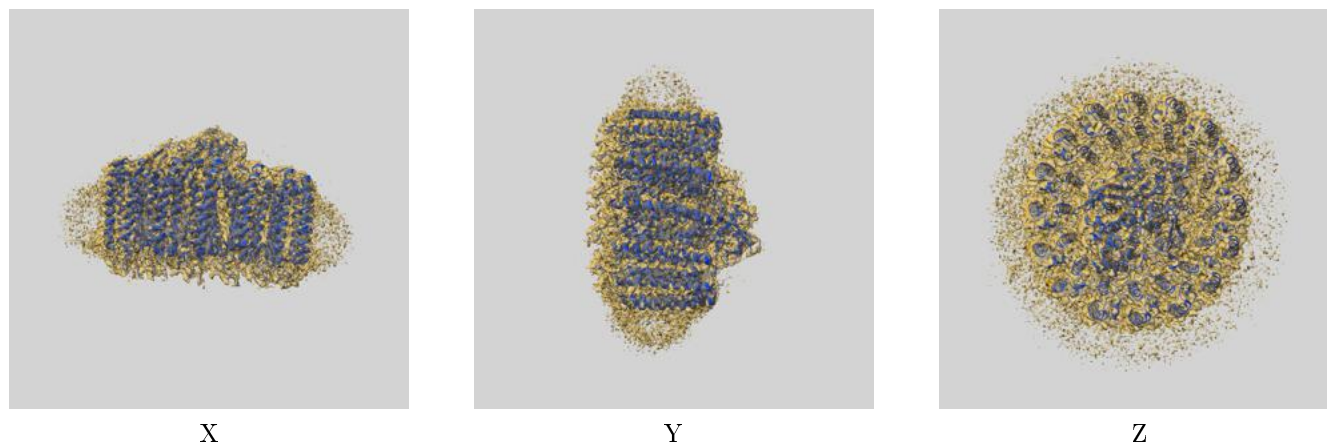
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.49	2.83	2.55
Unmasked-calculated*	-	-	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

## 9 Map-model fit [i](#)

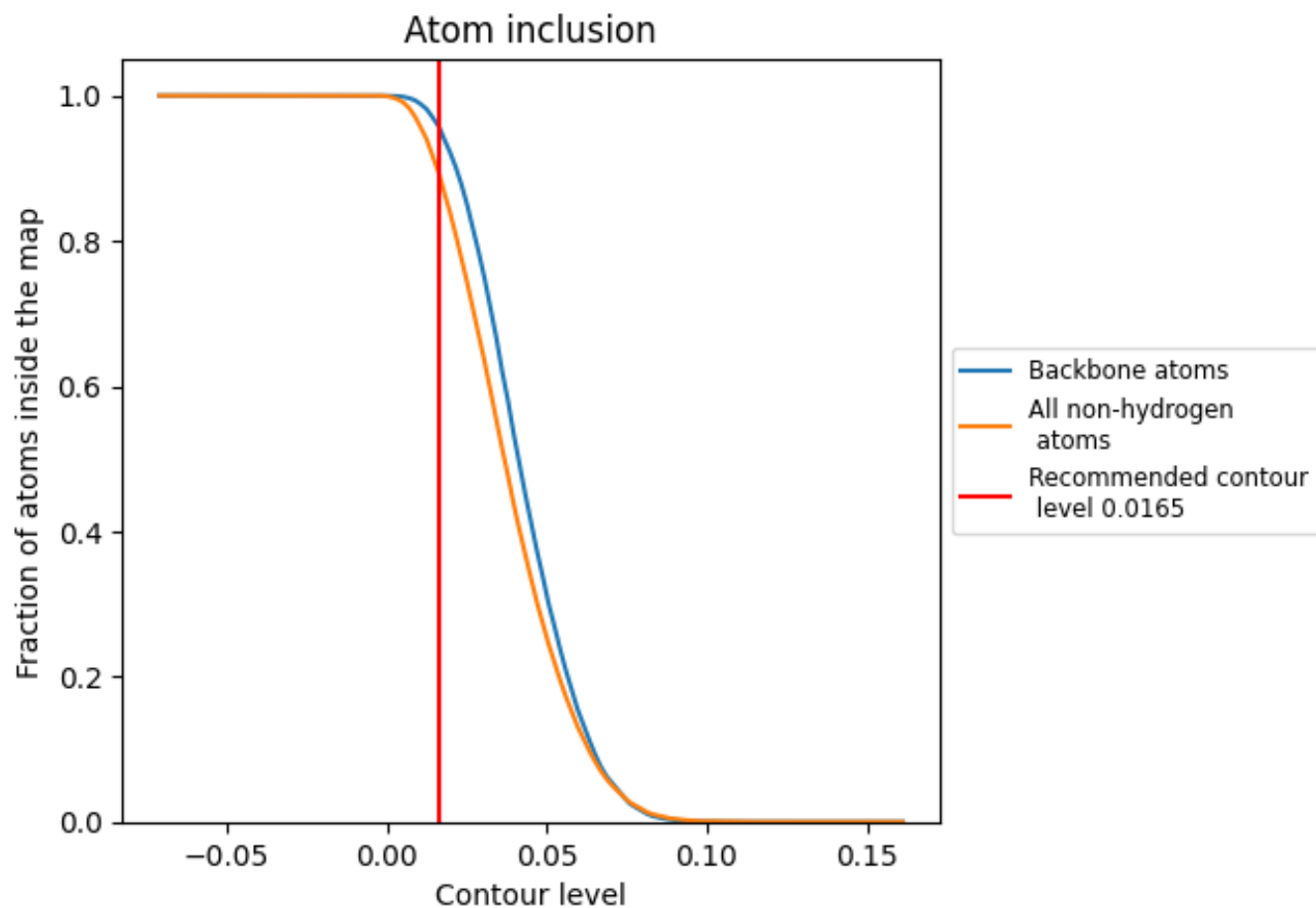
This section contains information regarding the fit between EMDB map EMD-13110 and PDB model 7OY8. Per-residue inclusion information can be found in section 3 on page 19.

### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.0165 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.